Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020101

FWP and possible subtask under FWP: Structure and Phase Transformations of Nanophases Embedded in Solids
FWP Number: KC11A

Program Scope: This program is aimed at understanding the fundamental features that underlie the behavior of nanoscale phases embedded in a solid matrix and their role in the evolution of microstructure in materials. Because of the scale and nature of such microstructures, electron microscopy is an integral part of these investigations - as an analytical tool as well as a subject of technique development. The fundamental principles established using model alloy systems are employed in the design and testing of new materials such as Al-based alloys of interest for energy-related technologies. The long-term objective is to develop an understanding of individual embedded nanostructures as a function of their size, shape and embedding parameters such as elastic strain and crystallographic alignment. This understanding will be critical for the application of nanomaterials because it addresses the fundamental question of their interaction with a solid environment.

Major Program Achievements (over duration of support):

By combining high resolution electron microscopy with 3D atom probe (ShaRE Program at ORNL) we have been able to confirm directly the hypothesis of pre-precipitation clustering driven by strain compensation. The electron microscopy data showed that clusters had not yet transformed to the diamond cubic structure of precipitates while the atom probe proved that clusters contained both Si and Ge. Similar clusters were absent in binary alloys.

We were able to synthesize nanocomposite alloy films of Al-Mo far from equilibrium by using room temperature co-sputtering. A systematic investigation of microstructure and properties as a function of Mo content resulted in an optimum film composition of Al-32at%Mo with a unique microstructure comprised of a dense distribution of nm-scale Mo crystallites dispersed in an amorphous Al-rich matrix. These films were found to exhibit unusually high nanoindentation hardness and a very significant reduction in roughness compared to pure Al, while maintaining resistivity in the metallic range, making them ideal materials for NEMS device applications.

A comparative TEM-based analysis of precipitation in binary and ternary alloys of Al with Sc and Zr has confirmed that Zr reduces coarsening by forming a Zr-rich shell, about 7nm in thickness, around a Sc-rich core of coherent precipitates. Isothermal heat treatments demonstrated this core-shell structure to be extremely stable over long periods of aging.

Program Impact:
This work has led to an improved understanding of the key role played by embedding parameters in the evolution of microstructures. In particular, the role of crystallographic alignment and confinement in a solid matrix on the behavior of nanoscale particles has been elucidated and utilized in thin film growth and precipitation reactions.

Interactions:
University of Alberta (D. Mitlin)
Centro Atómico Bariloche (A. Tolley)
ORNL (M. Miller)
LLNL (P. Turchi)

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Over 20 Invited talks since 2003
Personnel Commitments for FY2006 to Nearest +/-10%:
U. **Dahmen** (group leader) 5%, V. Radmilovic (staff scientist) 50%, A. Tolley (visiting researcher) 30%.

Authorized Budget (BA):

FY04 $204K	FY05 $204K	FY06 $192K

Laboratory Name: Lawrence Berkeley Nat. Laboratory
B&R Code: KC020102

FWP and possible subtask under FWP: Mechanical Properties of Advanced Materials Program
FWP Number: KC13

Program Scope:
A multidisciplinary investigation of the mechanical properties of advanced materials, involving interface composition, structure/bonding and mechanical properties provides new comprehension of materials architecture at multiple length-scales (from atomic to macro-scale) that can motivate development of superior ceramics and composite materials and related interfacial structures. Specifically, boundaries and dissimilar interfaces are evaluated and results related to interface-dictated properties, including mechanical and thermo-chemical stability, kinetic and dynamic behavior.

Major Program Achievements (over duration of support):
A set of *in situ* toughened ceramics, ABC-SiC, with excellent toughness, creep, wear and fatigue strength to 1400°C was developed. Corollary results include: elucidated how additives dictate derived grain morphology and character of the nanoscale intergranular films (IGFs), that are critical to achieving superior cold to hot behavior in SiC and Si_3N_4; correlated properties with atomistic computations and continuum modeling of IGF structure, stability and properties; assessed the atomic location and bonding of additives in Si_3N_4 IGFs via STEM imaging; and determined important, but rarely known worst-case cracking thresholds, intrinsic toughnesses and short crack R-curves for several ceramics.

Developments in processing include (i) SiC ceramics containing Al, B, C (ABC-SiC) synthesized by free-sintering, with roles of temperature and sintering atmosphere assessed. A range of rare-earth dopants introduced to modify systematically the IGF compositions formed, and to determine their effect on mechanical properties. Experiments backed by first-principle calculations, using the NERSC computation facility, relating structure and composition of IG Al-O-C clusters to grain-boundary adhesion and fracture of ABC-SiC, (ii) development of an ice-templating processing technique that manipulates the ice microstructure to make bio-inspired composite structures, with exceptional mechanical properties, and (iii) novel transient-liquid phase-based methods for joining ceramics that exploit multilayer, microdesigned interlayers, e.g., joining Al_2O_3 with a dewetting liquid-film using Cu/Nb/Cu.

Interface chemistry and structure directly related to strength and toughness several Al_2O_3/ metal/multilayers, including Al_2O_3/(M-Al) alloy interfaces from high-temperature oxidation, the latter entailing void formation, oxide layer growth, with S interface adsorption/adherence depending strongly on alloy content.

A suite of signature model experiments were implemented to assess the energetics of ceramic surfaces and influences of surface anisotropy on morphological evolution. A hierarchy of controlling mechanisms for reactive spreading of liquids was identified and illustrated including: new model derived for ridge-limited liquid spreading at high temperature, atomic mechanisms controlling rapid liquid-metal spreading prior to nucleation of triple line ridges, and identification of surface-tension driven (Marangoni) films in metal-metal systems.

Program Impact: While developing a tunable family of SiC-based ceramics with unparalleled cold strength and toughness with hot creep/fatigue properties, new strategies established for material optimization, i.e., by exploiting reversible changes in interface structure via heat treatment to assess key mechanical properties, including a new concept, the *fatigue threshold R-curve*. Hitherto unknown multiple segregation regimes at dynamic Al_2O_3/alloy interfaces related to alloy composition and oxide phase. Radical re-evaluation of the classic Young-Dupré equation for contact angle/wetting behavior of high temperature liquids plus novel mechanistic analysis yields a breakthrough in conceiving liquid spreading at high temperatures.

Interactions:
Internal— Advanced Light Source, National Center for Electron Microscopy, NERSC computation facility
External—ORNL; LLNL; SNL; ANL; LANL; IEENL; NIST; MIT; CMU; Crystal Systems Inc.; MPI Stuttgart.

Recognitions, Honors and Awards (at least in some part attributable to support under this program):
R.O. Ritchie – Wöhler Medal (European Structural Integrity Society); Xun Kee Lecture Award (IMR, China)
A.P. Tomsia – elected as one of 2006 *Scientific American's* 50 (Technology Leaders) awards

Personnel Commitments for FY2006 to Nearest +/- 10%:
R. O. Ritchie (10%), J. W. Ager (10%), L. C. DeJonghe (10%), A. M. Glaeser (15%), P. Y. Hou (50%), E. Saiz (50%), A. P. Tomsia (20%)

Authorized Budget (BA):

FY04 $1321K	FY05 $1314K	FY06 $1161K

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020103

FWP and possible subtask under FWP: Electronic Materials Program
FWP Number: MSD KC1201

Program Scope:
The Electronic Materials Program advances the fundamental understanding of the materials science of semiconductors. The research focuses on the relationships between synthesis and processing conditions and the structure, properties, and stability of semiconductor materials systems. Progress in these areas is essential for the performance and reliability for technologies that lie at the heart of the DOE mission including ultrahigh efficiency photovoltaic energy conversion devices, high efficiency solid-state sources of visible light, visual displays, and of a large variety of sensors and power control systems for energy generation, conservation, distribution and use.

Major Program Achievements (over duration of support):
- Pioneered scientific applications of isotopically controlled semiconductors; performed definitive impurity and self diffusion studies in Group IV and III-V semiconductors using stable enriched isotope superlattices.
- Developed new theory (band anticrossing model) to explain properties of "highly mismatched" alloys (HMAs) such as GaN_xAs_{1-x} and discovered new II-VI-based HMAs, including the first multiband semiconductor.
- Contributed significantly to the understanding of InN as a narrow gap semiconductor.
- Pioneered the use of pulsed laser melting for the synthesis of highly non-equilibrium alloys, including HMAs and "spintronic" materials.
- Established fundamental relationship between native defects and the achievable limits for doping.
- Identified Mn interstitials as the crucial defects in ferrmomagnetic $Ga_{1-x}Mn_xAs$ and established that these defects lead to a thermodynamic limit on the Curie temperature in this alloy system.
- Developed advanced electron microscopy methods to quantify the growth mechanisms of extended defects and to determine the atomistic core structure of dislocations in group III nitride thin films and heterostructures.

Program Impact: Under sustained BES funding, the Electronic Materials Program has discovered new classes of semiconducting materials (e.g., II-VI HMAs) and has contributed significantly to the synthesis and fundamental understanding of a large number of elemental and compound semiconductors. Basic research in the Program concerning the interplay of extended defects, compositional fluctuations, and the resulting strain distributions and the light emission mechanism in GaN and InGaN aided the development of solid-state lighting based on this materials system. Most recently, Program research has established that both In-rich InN and certain II-VI and III-V HMAs show promise as entirely new types of high efficiency solar cells and other opto-electronic devices.

Interactions:
Internal—National Center for Electron Microscopy, Advanced Light Source.
External—Hewlett-Packard, Agilent, MPI Stuttgart, Xerox, NREL, Cornell, Purdue, Notre Dame, MIT, Harvard, Münster Univ., Germany, Inst. High Pressure Physics, "Unipress", Georgia Tech.

Recognitions, Honors and Awards (at least in some part attributable to support under this program):
J. W. Ager III – co-author, "Isotopic Effects in Solids," *Encyclopedia of Condensed Matter Physics*,
co-editor, Topical Issue of *Semiconductor Science and Technology*, "Group III-N-V Alloys," 2002.
O. D. Dubon – Presidential Early Career Award for Scientists and Engineers (PECASE), 2004.
E. E. Haller – Turnbull Award, MRS, 2005; Fellow of AAAS, 2004; James C. McGroddy Prize for New Materials of the American Physical Society, 1999; Chair, 20th Intl. Conf. on Defects in Semiconductors, Berkeley, CA 1999; Max-Planck Research Award, 1994; Research Professor, Miller Foundation for Basic Research in Science, 1990 and 2001; Fellow, American Physical Society, 1986; A. von Humboldt US Senior Scientist Award, 1986.
Z. Liliental-Weber – Chair, IEEE Semiconducting and Insulating Materials Conference, Berkeley, CA 1998.
W. Walukiewicz – Fellow, American Physical Society 2006; R&D 100 Award, 2006; Chair, Gordon Res. Conf. on Defects in Semiconductors 2006; co-editor, Topical Issue of *Semiconductor Science and Technology*, "Group III-N-V Alloys," 2002, NTT distinguished Professorship 1990.
E. R. Weber – Fellow, American Physical Society, 2001; Humboldt Senior US Scientist Award, 1994.
K. M. Yu – R&D 100 Award, 2006.

Personnel Commitments for FY2006 to Nearest +/- 10%:
E. E. Haller (20%), J. W. Ager III (40%), D. C. Chrzan (10%), O. D. Dubon, Jr. (10%), Z. Liliental-Weber (60%), W. Walukiewicz (80%), E. R. Weber (10%), K. M. Yu (60%).

Authorized Budget (BA):
FY04 $1392K FY05 $1348K FY07 $1410K

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020103

FWP title and possible subtask under FWP: Mechanics at Hard-Soft Materials Interfaces
FWP Number: KC1202

Program Scope: The overall program goal is to advance the fundamental understanding of complex phenomena in soft and hard materials. The research focuses on two areas: (i) understanding of transport of liquids, ions, and biomolecules in ***nanofluidic*** channels: This explores a new class of nanomaterials to study molecular and ionic transport in confined or low-dimensional liquids. (ii) understanding the chemomechanics of reaction-induced mechanical forces, and using it for biological and chemical sensing and actuation.

Major Program Achievements (over duration of support):

- Showed that the ionic conductance in nanochannels is about 10^4-10^5 times higher than predicted by bulk theory.
- Created the first nanofluidic transistor and demonstrated transconductance
- Demonstrated digital control of protein transport in transistor circuits
- Demonstrated an interesting ionic transition during DNA translocation and protein reaction in fluidic nanotubes/nanochannels and showed that it can be used to measure the charge-to-volume ratio of biomolecules
- Experimentally demonstrated nanoscale patterning of molecules inside nanofluidic channels and developed the appropriate reaction-diffusion theory to predict the behavior
- Observed novel phase transition phenomena in nanofluidic channels, which seem to resemble spinodal decomposition
- Developed micro-cantilever and micro-membrane arrays for studying nanomechanics of molecular reactions in high-throughput manner.
- Developed surface chemistry protocols for attachment of biomolecules and preventing biomolecules from nonspecific binding
- Using directed evolution of bacteriophages, created new receptors for small molecules such as DNT and TNT
- Developed sensor system for portable chemical sensor

Program impact: The impact of studying aqueous solutions of ions and biomolecules could have significant impact on fundamental understanding of water, with implications in water purification, biochemical assays at possibly single cell levels, and electrochemical energy conversion/storage. The development of highly selective receptors for important gas molecules, and then their utilization in chemical sensing addresses a fundamental national need.

Interactions:
Peidong Yang (Dept. of Chemistry, UCB and MSD, LBL); Arup Chakraborty (Depts. of Chem. Engr & Chemistry, UCB and MSD, LBL); Frank Chen (Life Sciences Division, LBL); Ron Zuckermann (Chiron Corp.), Seung-Wuk Lee (Dept. of Bioengineering, UCB and MSD, LBL)

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
(i) Elected to National Academy of Engineering; (ii) Member, Nanotechnology Advisory Group, President's Council of Advisors on Sci. & Tech. (PCAST); (iii) Member, Council of Materials Science & Engineering, DOE; (iv) Member, Advisory Committee, Engineering Director of NSF; (v) Heat Transfer Memorial Award; (vi) 20 Academic Invited Talks; 12 Conference Invited Talks; 3 Industry Invited talks.

Personnel Commitments for FY2005 to Nearest +/- 10%: (provide name where relevant)
Arun Majumdar (PI): 10 %
2 Graduate Student: 49.5% 9 month academic year + 100 % 3 month summer (one working on nanofluidics and the other working on peptoids)

Authorized Budget (BA):

FY04 $230K	FY05 $230K	FY06 $230K

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020103

FWP and possible subtask under FWP: Characterization of Functional Nanomachines

FWP Number: MSD KC1203

Program Scope:
Development and application of controllable, operational nanomachines and nanomotors from molecular building blocks. Determination and control of the mechanisms of chemical-to-mechanical energy transfer in naturally occurring molecular biomotors, artificial biomotors, and engineered biochemical assemblies. Chemical synthesis of new molecules having tailored geometry, electro-activity, and surface reactivity for use as nanomachine components. Local probe study of functional molecules adsorbed to surfaces and actuated using optical and electronic stimulous. Use of combined MEMS technology and fullerene growth techniques to create electro-mechanically actuated molecular motors from carbon nanotubes. Theoretical prediction and explanation of nano-motor behavior through *ab initio* electronic structure calculations.

Major Program Achievements (over duration of support):
Observation of reversible photomechanical switching of single-molecules at a surface using azobenzene derivatives. Use of nano-droplet surface tension to create new nanoscale relaxation oscillator. Synthesis and testing of nanotube nanomotor arrays. *ab initio* calculation of electronic structure of *cis* and *trans* states of photomechanically active molecules, new predictions of excited state dynamics of adsorbed azobenzene molecules. Characterization of friction and dissipation of interlayer nanotube bearings. Determination of new mechanisms for mechano-chemical transduction in the packaging motor of bacteriophage phi29, directional translocation on DNA by the protein machine FtsK, and supercoiling action of *E. coli* gyrase. Development of new tip-activated reaction-based lithography technique to create chemically active surface patterns using amine-based chemistry of SAMs on silicon.

Program impact:
First observation of reversible, light-activated single-molecule switch. Fabrication and operation of remotely controlled nanotube-based mechanical motors capable of operation at high and low temperature and in vacuum environment. Control of molecular nanomechanical and self-assembly behavior at surfaces. Theoretical understanding of mechanical energy dissipation mechanisms (friction) in nanotube bearings. Significant progress in characterizing and re-engineering naturally occurring molecular machines and biomotors.

Interactions:
Internal: National Center for Electron Microscopy, National Scientific Computing Center (NERSC), Advanced Light Source, Berkeley Microfabrication Laboratory
External: IBM Almaden, Yale, University of Vienna, Max Planck Institute Stuttgart, University of Pennsylvania, Pennsylvania State University, UCLA, SUNY Stony Brook, Seoul National University, Korea, Hong Kong University of Science & Technology, and Universidad del Pais Vasco, Spain

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
A. Zettl - R & D 100; **M. L. Cohen** - National Medal of Science, APS President; **Carlos Bustamante -** Honorary Degree Doctorate by the University of Chicago**; J Frechet** - 2005 Esselen Award for Chemistry at the Service of Society; **S.G. Louie** - National Academy of Science, Outstanding Overseas Chinese Award; **D. Trauner** - Novartis Young Investigator Award

Personnel Commitments for FY2005 to Nearest +/- 10%:
1 Principal Investigator (Crommie (35%))
6 faculty scientists (Bustamante (15%), Cohen (10%), Frechet (15%), Louie (10%), Zettl (20%), Trauner (20%))
5 postdocs (A. Kirakosian (50%) R. Case (100%), T. Hugel (10%), P. Zhang (50%), S. Aloni (50%))
6 grad. students (M. Comstock (100%), K. Sivula (35%), A. Murphy (100%), G. Begtrup (60%), J. Sau (50%), M. Volgraf (100%))

Authorized Budget (BA):
FY04 $647K **FY05** $939K **FY06** $920K

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020103

FWP and possible subtask under FWP: Nanowire-Based Functional Devices and Assemblies
FWP Number: KC1204

Program Scope: The goal of this research is to develop the science and technology of a broad spectrum of 1-dimensioanl inorganic semiconducting nanostructures or nanowires for energy-related applications. Our approach relies on the vapor-liquid-solid (VLS) process that can be used to grow monocrystalline nanowires Si, Ge, SiGe, GaN, ZnO and various II-VI, III-V semiconductors and their alloys. Significant research efforts have been placed on the fundamental understanding and control of the nanowire nucleation/growth. The fundamental information is then be used to guide the nanowire growth process which would include monodispersity control over size and aspect ratio; growth orientation control, precise site control and accurate density control. Lastly, both parallel process (Langmuir-Blodgett technique) and serial process (nanomanipulation, optical trapping) are being explored for the hierarchical assembly of these nanowire building blocks for their potential nanophotonic and energy conversion applications. The potential of using these semiconductor nanowires for photonics, solid state lighting, photovoltaics and thermoelectrics are being actively investigated.

Major Program Achievements (over duration of support):
(1). The development of on-chip photonic sensors requires novel materials that control the flow of light through liquids with structures smaller than the wavelength of the light guided. We have demonstrated a novel optical sensing platform that utilizes the evanescent field of a single-crystalline nanoribbon waveguide to perform absorbance, fluorescence and surface enhanced Raman spectroscopy (SERS) on sub-picoliter volumes of solution. We obtain the chemical specificity of SERS by decorating the waveguide with silver nanocubes to enhance the field around the nanoribbon. These results open up the possibility of engineering hand-held, photonic sensors capable of detecting and identifying chemical species in solution.
(2). Recent advances in nanomanipulation have made it possible to modify the shape of these structures from a linear to a pseudo–ring conformation. Changes to the optical boundary conditions of the lasing cavity affect the structure's photoluminescence, photon confinement, and lasing as a function of ring diameter. For a given cavity, ring-mode red-shifting is observed to increase with decreasing ring diameter. Significant shifts, up to 10 nm for peak emission values, are observed during optical pumping of a ring resonator nanolaser compared to its linear counterpart. The study allows the mode-spacing and position to be tuned with the same nanowire gain medium.
(3). We have demonstrated that an infrared single-beam optical trap can be used to individually trap, transfer, and assemble high-aspect-ratio semiconductor nanowires into arbitrary structures in a fluid environment. Nanowires with diameters as small as 20 nm and aspect ratios of above 100 can be trapped and transported in three dimensions, enabling the construction of nanowire architectures which may function as active photonic devices. Moreover, nanowire structures can now be assembled in physiological environments, offering novel forms of chemical, mechanical, and optical stimulation of living cells.

Program Impact: Develop the science and technology of a broad spectrum of 1-dimensioanl inorganic semiconducting nanostructures or nanowires for energy-related applications including nanophotonics and energy conversion.

Interactions: Arun Majumdar; Richard Saykally, Jan Liphdart.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):

2006	Molecular Science Forum Professorship, Institute of Chemistry, Chinese Academy of Science.
2006	Yangtze Scholar, Chinese Ministry of Education
2006	McElvain Lectureship, Department of Chemistry, University of Wisconsin, May, 2006.

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Personnel Commitments for FY2006 to Nearest +/-10%:
P.D. **Yang** (PI) 20%**;** Don Sirbuly (Postdoc) 100%; Wenjie Liang (postdoc) 50%, Peter Pauzauskie (Graduate student) 100%.

Authorized Budget (BA):

FY04 $0K	FY05 $411K	FY06 $411K

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020103

FWP title and possible subtask under FWP: Nanostructured Materials for Thermoelectric Energy Conversion
FWP Number: KC1205

Program Scope: The overall program goal is to investigate the basic science of thermoelectricity and phonon transport in nanostructured materials in order to gain fundamental understanding of how thermopower, S, electrical conductivity, σ, and thermal conductivity, k, can be manipulated independently so that the thermoelectric figure of merit, $ZT = S^2\sigma T/k$, can be maximized. In order to do so, the program focuses on three classes of materials: (i) hybrid organic-inorganic heterostructures; (ii) complex oxides; (iii) bulk semiconductor nanostructures such as arrays and assemblies of nanowires, nanoholes, and nanoparticles in bulk materials.

Major Program Achievements (over duration of support):

- Developed a new statistical method for estimating the electrical conductance of single molecules
- First measurement of the thermopower of single molecule heterojunctions
- First measurement of the thermal conductance of molecular monolayers
- Thermal conductivity reduction by a factor of 5 in nanoparticle embedded complex oxides
- Demonstrated unusually high thermopower in SrLaTiO films
- Demonstrated power factors ($S^2\sigma$) in SrLaTiO films that are comparable to the best BiTe materials
- New synthesis technique for making Si nanowire arrays at the wafer scale by etching
- Thermal conductivity reduction by a factor of about 100 in etched Si nanowires without reduction of power factor
- Demonstrated increase in ZT by 20 percent in nanoparticle embedded BiTe bullk materials.

Program impact: Direct thermal to electrical energy conversion using solid-state thermoelectric devices is attractive because such devices contain no moving parts and are environmentally benign, and produce electricity from waste heat. If it is used world wide to recover waste heat, it could produce about 400 GW of electric power, which is approximately one half the capacity of USA. Furthermore, it could used for refrigeration as well. What prevents its widespread use are: (i) performance; (ii) cost effectiveness. Currently, their performance is below 10 percent of the Carnot limit. While five decades of research has led to understanding of the basic attributes of a bulk thermoelectric material, there is no clear roadmap of increasing $ZT = S^2\sigma T/k$ from 1 to 3. If successful, this program could produce new materials that could increase ZT while simultaneously making them cost effective.

Interactions:
Arun Majumdar (Depts of Mechanical Engr & Materials Science and Engr., UCB and MSD, LBL); Peidong Yang (Depts. of Chemistry and Materials Science & Engr., UCB and MSD, LBL); Joel Moore (Department of Physics, UCB and MSD, LBL); Ramesh Ramamoorthy (Departments of Materials Science & Engr and Physics, UCB, and MSD, LBL); Rachel Segalman (Dept. of Chemical Engr., UCB and MSD, LBL)

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Majumdar: Elected to National Academy of Engineering, Member-Nanotechnology Advisory Group, President's Council of Advisors on Sci. & Tech. (PCAST), Member-Council of Materials Science & Engineering-DOE, Member-Advisory Committee-Engineering Director of NSF, Heat Transfer Memorial Award; 20 Academic Invited Talks, 12 Conference Invited Talks, 3 Industry Invited talks. *Ramesh:* Fellow-AAAS, Adler Lectureship-APS. *Yang:* Pure Chemistry Award-ACS, Cmille Dreyfus Teacher-Scholoar Award, 100 Top Young Innovators-MIT Tech. Review, TR100 Award-Tech. Review, Beckman Young Investigator.

Personnel Commitments for FY2005 to Nearest +/- 10%: (provide name where relevant)

Authorized Budget (BA):

FY04 $___K	FY05 $550K	FY06 $550K

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020103

FWP and possible subtask under FWP: Spin Functionality through Complex Oxide Heteroepitaxy

FWP Number: KC1206

Program Scope: Development of highly spin polarized thin film materials that will shed light on key unresolved questions in magnetism concerning the nature of magnetism at boundaries of spin-polarized materials and that will facilitate more energy efficient spin-based electronic applications. We are developing novel functional oxide thin films and heterostructures with spin polarized functionality in order to: (i) design and synthesize complex oxide thin film materials with spin polarized functionality; (ii) obtain a fundamental understanding of the nature of magnetism at boundaries; (iii) develop close collaborations with colleagues at Lawrence Berkeley National Lab (LBNL), Argonne National Laboratory (ANL) and other DOE labs; (iv) act as a resource for thin film materials development; (v) train the next generation of scientists in thin film materials synthesis at the undergraduate, graduate and postdoctoral levels.

Major Program Achievements (October 2005 to September 2006):
Magnetic Oxide Nanostructures: Developed novel process for the fabrication of complex magnetic oxide nanostructures where magnetic domain structure can be tuned by shape, crystal structure and strain effects. Highly spin polarized complex magnetic oxide nanostructures embedded in a paramagnetic matrix have been fabricated, for the first time, by electron beam lithography and ion implantation. Imaging the magnetic domains with X-ray photoemission electron microscopy and magnetic force microscopy reveal a delicate balance between magnetocrystalline, magnetoelastic, and magnetostatic energies that can be tuned by the choice of $SrTiO_3$ substrate orientation, film thickness, island size, and island shape.
Oxide junction heterostructures: Developed an understanding of magnetism at oxide interfaces and novel spin dependent transport mechanisms in oxide junction heterostructures based on spinels and perovskites. Our studies of Fe_3O_4 and $La_{0.7}Sr_{0.3}MnO_3$ based junctions indicate that depending on temperature and bias, elastic tunneling or inelastic hopping dominates along with surface magnons from the electrodes or bulk magnons from the barrier. These junctions provide a model system for a novel type of hybrid spin filter/magnetic tunnel junction device.
Novel oxide interface materials: Developed thin film processing methods to synthesize oxide heterostructures with an in-situ X-ray scattering probe.

Program Impact:
The development of complex oxide thin film materials with spin polarized functionality has provided model systems which shed light on the nature of magnetism at boundaries of spin-polarized materials. Understanding spin polarization at these surfaces and interfaces is a key element in the development of a more energy efficient spin-based electronics.

Interactions:
Lawrence Berkeley National Laboratory, Advanced Light Source: Elke Arenholz, Andreas Scholl, Andrew Doran
Lawrence Berkeley National Laboratory, Molecular Foundry: J. Alex Liddle, Bruce Harteneck
Argonne National Laboratory, Materials Science Division: J.F. Mitchell, H. Zheng
Cornell University and Cornell High Energy Synchrotron Source: Joel Brock, Darren Dale

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Advanced Light Source 2006 Users' Workshop Best Poster Award.

Personnel Commitments for FY2005 to Nearest +/-10%:
Note that funding started July 2005 for a total of 3 months for FY2005
Y. Suzuki (PI) 20% time for this project (paid 1 month summer salary during August 2006)
Y. Takamura (post-doc) 100%
B.B. Nelson-Cheeseman 100% time on this project but paid for 0% time by DOE as she is on fellowship
Franklin Wong 100% time on this project but on fellowship during '05-'06 academic year

Authorized Budget (BA):
FY04 $0K FY05 $250K FY06 $250K

Laboratory Name: Lawrence Berkeley Nat. Laboratory
B&R Code: KC020103

FWP and possible subtask under FWP: Nanocomposite Proton Conductors
FWP Number: KC13H

Program Scope:
The program aims to design, synthesize and test rare earth phosphate materials for proton conducting applications in the temperature region of 300-450 degrees Celsius. The program relies on three major approaches: a theoretical understanding of proton conduction in rare earth phosphates employing quantum chemical computation and molecular simulation; the chemical design, synthesis, and proton conductivity measurement of nano-composite materials expected to exhibit facile proton conduction; and the structural and dynamical characterization of the nano-composite materials using a range of advanced characterization methods including high resolution TEM, computational methods, as well as nuclear magnetic resonance (NMR). Aliovalently-substituted rare earth phosphates and rare earth phosphate glasses are being synthesized and tested for proton conduction. A comparison of theoretical predictions and observed conductivities provides an insight into the microscopic nature of conduction and directs the synthesis of novel nano-composite rare earth phosphates with modified grain boundaries.

Major Program Achievements (over duration of support):
Synthesized and characterized nano-composite Lanthanum and Cerium phosphates with modified grain boundaries. Developed a theoretical model for proton conduction in rare earth phosphates using computational chemistry and dynamic simulations methods.
Explored the structural and functional characteristics of the grain boundaries with TEM, EDAX and NMR, revealing the formation of highly conductive amorphous phases. Directed the findings towards the design and synthesis of rare earth glasses for proton conduction.

Program Impact:
Proton conductors operational in 300-450 ^{o}C have tremendous potential as fuel cell membranes, hydrogen separation membranes and sensors, etc. In addition, to possibility of membrane forming methods similar to those of the glass industry offer considerable economic advantage. It has been demonstrated that a careful combination of the structural characteristics of highly conductive amorphous phases and the structurally stable crystalline rare earth phosphates can result in the formation of materials with enhanced proton conduction at elevated temperatures. The preparation and characterization of pure and doped rare earth phosphate glasses is very valuable to an understanding of the functional properties of inter-granular boundaries in the nano-composite materials.

Personnel Commitments for FY2006 Nearest +/- 10%:
De Jonghe(10%), Reimer(10%), Ross(10%), 4 postdocs(100%), 4 students (100%)

Authorized Budget (BA):
FY04 $0K FY05 $850K FY06 $850K

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020202

FWP and/or subtask Title under FWP: Superconductivity
FWP Number: MSD KC2201
Program Scope: Development of low-and high-transition temperature (T_c) Superconducting QUantum Interference Devices (SQUIDs) and their application to a broad range of phenomena. Low-T_c SQUIDs: nuclear magnetic resonance (NMR) and magnetic resonance imaging (MRI) in ultralow magnetic fields at frequencies as low as 100 Hz; novel microstrip resonator configuration for quantum-limited detection and readout of quantum bits. Studies of nanofabricated structures and devices. Specific-heat measurements used to investigate relations between structure and physical properties of materials, including superconductors.

Major Program Achievements: Noise reduced in microstrip SQUID amplifier by a factor of three by means of thin-film cooling fins that remove hot electrons inherent in readout of the device, and by reducing the coupling to the input and output circuitry. SQUID-detected magnetic resonance images obtained in zero applied magnetic field with novel pulse technique. Comprehensive theory of the rf SQUID amplifier has been developed taking into account the loading of the input and output circuitry, and shown to be comparable to that of the dc SQUID. Detailed theory for the "antiproximity effect" in superconducting nanowires demonstrates that the origin lies in dissipation in the environment. Properties of $Na_{0.3}CoO_2 \cdot 1.3$ H_2O shown to be affected by time-dependent pair breaking. Internal equilibration time shown to be a serious problem in relaxation calorimetry on nanomaterials; this problem had previously been generally overlooked. Measurements on BCN nanotubes show size and dimensionality effects.

Program Impact: (JC): Groups at LANL, PTB (Germany), Jülich (Germany) have constructed SQUID-based NMR and MRI systems. SQUID-multiplexers for readout of far infrared bolometers deployed on a 330-element array on a telescope at Atacama, Chile (funded by NSF). Axion detector at LLNL upgraded with microstrip SQUID amplifier (funded by DOE high energy physics). Microstrip SQUID amplifiers are in operation at Yale University, Chalmers University, Gothenburg, Sweden and the University of New South Wales, Australia for quantum-limited detection. (NEP): Measurements on $Na_{0.3}CoO_2 \cdot 1.3$ H_2O provide understanding of the "sample dependence" of properties.

Interactions: Internal: (JC): E.L. Hahn (Physics, UCB); B. Inglis, (Brain Imaging Center, UCB); A.T. Lee (Physics, UCB); D-H. Lee (Physics, UCB); J.W. Morris (MSD, LBNL and Materials Sciences, UCB); A. Pines (Chemistry, UCB and MSD, LBNL); P.L. Richards (Physics, UCB); H. Spieler (Physics, LBNL). (NEP): D-H. Lee (Physics, UCB); A. Zettl (Physics, UCB and MSD, LBNL).

External: (JC): P. Delsing (Chalmers University, Sweden); N. Hylton (UCSF); D. Kinion (LLNL); R.H. Koch, (IBM); J. Kurhanewicz (UCSF); M. Mück (University of Gießen, Germany); D. Reilly (University of New South Wales); R.J. Schoelkopf (Yale University); M. Shuman (UCSF); J. Simko (UCSF); K. van Bibber (LLNL). (NEP): Amherst College; Centre d'Études Nucléaires, Grenoble; LLNL, LANL; Max Planck Institut (Stuttgart); Princeton University.

Recognitions, Honors and Awards: (JC): Member of Solid State Sciences Committee of National Academy of Sciences (2003-2006). International Advisory Committee, MS+S 2006, Atsugi-shi, Japan; Co-Chair, MQC2-2006, Naples, Italy; International Advisory Committee, ISS, 2006, Nagoya, Japan. 30 invited talks in 2006. (NEP): Invited talk at First International Workshop on the Physical Properties of Layered Cobaltates, Orsay, July 2006.

Personnel Commitments for FY2006 to Nearest +/- 10%:
J. Clarke 15%; N.E. Phillips 75% (charged to project 5%) (program leaders); research chemist (25%): R.A. Fisher (charged to project 5%); gsr's (62.5%): W. Myers (graduated 5/06), N. Kelso, M. Hatridge, S. Busch, Daniel Slichter (started 1/06; charged to project 66% of year); postdocs (100%): D. Kinion (zero time charged to project), F. Hardy, M. Moessle; admin. (75%): B. Salisbury.

Authorized Budget (BA) for FY04, FY05, FY06:

FY04 BA $514K	FY05 BA $560K	FY06 BA $560K

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC20202

FWP and possible subtask under FWP: Quantum Materials Program
FWP Number: KC2202
Program Scope: "Quantum materials," systems in which the quantum-mechanical correlations of electrons play a dominant role, manifest a rich and diverse spectrum of physical phenomena. In materials such as the perovskite transition metal oxides for example, interacting charge, spin, orbital, and lattice degrees of freedom create a multi-dimensional phase space that make possible novel phases of matter and new functionalities. At LBNL we are ideally positioned to exploit the potential of these versatile materials because of the presence of a team of researchers with strongly overlapping interests and synergistic capabilities. We are carrying out a research program in which fundamental understanding of the novel phases and elementary excitations of bulk crystalline transition metal oxides serves to inform and guide our development of new functionality in oxide heterointerfaces and other artificially prepared nanostructures. The core QM team consists of Birgeneau, Lanzara, Lee, Orenstein and Ramesh. We collaborate with other members of the MSD and LBL community (Vishwanath, Hellman, Dahmen, Suzuki, Scholl, Rotenberg, Kortwright, Moore, Chrzan) to leverage the investment into this interdisciplinary effort.
Major Program Achievements (over the duration of the program): This is a newly funded program, which formally started 1 October 2006. Some of the PI's within this program have been funded individually in the past. Further, this program was funded as a LBNL-LDRD last year. Some of the accomplishments are outlined here. (i)We have probed the magnetism and transport in epitaxial $La_{1.2}Sr_{1.8}Mn_2O_7$ thin films synthesized in a wide range of deposition conditions. With the (110) orientation, the $La_{1-x}Sr_xMnO_3$ bilayers lie perpendicular to the substrate plane with the *c*-axis in the plane of the film, allowing us to measure the magnetic and electronic anisotropy of the material in a single sample. The thicker films possess bulk-like properties with a ferromagnetic transition that coincides with a resistivity maximum at a reduced T_c~90 K (vs. 120 K in bulk) and an anisotropy ratio, ρ_c/ρ_{ab}~20-200 over the range of 5-380 K. (ii) Orenstein and Ramesh are collaborating on understanding spin dynamics in a model correlated system, SrRuO3. In epitaxial thin films, the optical measurements show the existence of a clear ferromagnetic resonance at a relatively high frequency of ~250GHz. The collaboration between Ramesh, Suzuki and Orenstein is focused on exploring new classes of correlated materials with the potential for multiferroic behavior, such as vanadium-based perovskites. Structural analysis of the $PbVO_3$ thin films using transmission electron microscopy (NCEM), XRD and RBS reveal that the films are single tetragonal phase. Electron energy loss spectroscopy (**NCEM**) and x-ray absorption spectroscopy(**ALS**) were used to show the stabilization of the V^{4+} state, thereby proving the creation of a new d^1 system for intensive physical study. (iii) The theoretical work of Moore and Vishwanath addresses electrical and thermal transport at a two-dimensional quantum phase transition into a superconducting phase. The relevance of this work to the new two-dimensional electron systems to be created as part of this program is threefold. First, it required development of new numerical and analytical methods in order to access thermal and electric transport properties of a quantum critical electronic system. Second, the particular transitions studied here may be realized in doped Mott insulator heterostructures. Finally, this project highlighted the importance of thermoelectric and thermal transport as a tool to studying correlated systems and laid out the formalism for calculating these in other situations. Work is currently focused on modeling the correlated two-dimensional electron system using adaptations of standard correlated electron models to oxide nanostructures.
Recognition, Honors, and Awards (at least partly attributable to support under this FWP or subtask): *Ramesh:* Fellow-AAAS, Adler Lectureship-APS; *Lanzara:* Sloan Fellow, Hellman Faculty Fund award-UCB, NSF Career Award, McMillan Award-UIll/Champaign; *Majumdar:* Elected to National Academy of Engineering, Member-Nanotechnology Advisory Group, President's Council of Advisors on Sci. & Tech. (PCAST), Member-Council of Materials Science & Engineering-DOE, Member-Advisory Committee-Engineering Director of NSF, Heat Transfer Memorial Award; 20 Academic Invited Talks, 12 Conference Invited Talks, 3 Industry Invited talks; *Vishwanath:* Sloan Fellow.
Personnel Commitments +/10%: Orenstein 35%, Ramesh 10%, Vishwanath 20%, Lanzara 20%, Lee 15%. Postdocs and students to be hired in FY07 = 9 FTE.
Relationship to other projects. The Quantum Materials program is highly leveraged in terms of interdisciplinary collaborations within LBL as well as outside (i.e., other national labs and academic institutions). A significant component of our research is carried out in collaborations with scientists at the ALS. Suzuki, Lanzara and Ramesh are key users of various beamlines at the ALS for magnetic studies of complex oxide heterostructures and nanostructures as well as spectroscopy and collaborate extensively with Scholl, Arenholz, Rotenberg, and Kortright. Strong collaborations with scientists at the NCEM (Dahmen, Browning, Kieselowski, Schmid), in the area of energy loss spectroscopy and high resolution imaging of interfaces are already in place. We also have external collaborations with other National Labs (Argonne, BNL, ORNL) and academic institutions.
Authorizeed Budget (BA):

FY04 $428K	FY05 $678K	FY06 $728K

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020202

FWP and possible subtask under FWP: Ultrafast Materials Science
FWP Number: KC2203

Program Scope: Advanced ultrafast techniques applied to fundamental problems in condensed matter physics, including: (i) complex and highly-correlated materials exhibiting new physics, and (ii) exotic properties; and novel physics at surfaces, interfaces, and in nanostructured materials. Ultrafast THz, visible, and x-ray spectroscopy provides new insight to charge, spin, quasiparticle, and structure dynamics by separating correlated phenomena in the time domain. Ultrafast technology underpins unique nonlinear spectroscopies for probing surfaces and interface properties of liquids, polymers, and related solids.

Major Program Achievements: *Carrier dynamics in semiconductors*: scattering and dephasing dynamics demonstrated to be strongly dependent on system dimensionality, coherence of indirect excitons ideally-suited for creating a degenerate Bose-gas; elucidated dynamics of 2D electron gas (2DEG) in large magnetic field and influence of 2DEG on the coherence of *e-h* pairs in the quantum Hall regime; first observation of degenerate and spatially-ordered exciton states; first demonstration of THz stimulated emission from intra-exciton transitions; first measurement of spin diffusion coefficient of 2DEG and direct evidence of spin-Coulomb drag. *High-T_c Superconductors (HTS) and transition-metal oxides (TMO)*: pioneered research in THz optical conductivity of HTS including observation of optical Hall conductivity of quasiparticles and vortices; measurement of quasiparticle scattering in BSCCO revealing bimolecular kinetics of Cooper-pair formation; direct measurement of phase fluctuation rates of the superconducting (SC) order parameter and demonstration that they drive the SC/normal phase transition; first direct measurement of quasiparticle propagation (diffusivity tensor, and scattering rates) in a HTS; revealed the dominant band-like (v.s. Mott-Hubbard) character of the insulating state of VO_2; first evidence of an ultrafast insulator-metal transition (IMT) via vibrational pumping in PCMO. *Ultrafast x-ray science*: first demonstration of femtosecond pulses from a synchrotron; first time resolved x-ray spectroscopy of the ultrafast IMT in VO_2; first quantification of atomic displacements of coherent polariton mode in $LiTaO_3$; dynamic ligand dilation observed in ultrafast spin transition in TMO molecular complex. *Surface/Interface Physics*: new understanding of surface/interface properties of water, ice, and numerous other liquids and solids; pioneered the development of sum-frequency spectroscopy to study surface reactions under ambient conditions, and as a sensitive probe of molecular chirality with applications to *in-situ* study of biomolecules; developed powerful optical technique to study surface chemical diffusion of atoms and molecules with sensitivity to anisotropy, concentration, impurities, etc.

Program Impact: This program has generated new fundamental knowledge of electronic and atomic dynamics in condensed matter. Results from semiconductors, correlated electron systems, nanostructures, surfaces, and molecular complexes have challenged previously held assumptions and advanced new paradigms to describe the dynamic behavior that underpins novel material properties and functionality.

Interactions: Internal: LBNL Materials Science Div., Chemical Science Div., Earth Science Div., Advanced Light Source. External: U.C. Berkeley Physics Dept., Chemistry Dept., Stanford Univ., U.C. Santa Barbara, U.C. San Diego, U. Illinois, Michigan State, Naval Res. Lab., U. British Columbia, U. Tokyo, Tokyo Inst. Tech., CRIEPI Japan, Ecole Normale Superieure de Paris, Acad. Sinica Taiwan, Wietzmann Inst.

Recognitions, Honors and Awards (in part attributable to program support): *D. Chemla*: Member Nat'l Acad. Sci. (1997), Quantum Elect. Award (IEEE, 1995), Humboldt Prize (1995), Gordon Conf. Cruikshank Lecturer (1995); *J. Orenstein*: Chair Gordon Conf. on Correlated Elect. Sys. (2002-06); *R. Schoenlein*: Lomb Medal (OSA, 1992); *Y.R. Shen*: Townes Award (OSA, 1986); Schawlow Prize (APS, 1992); Distinguished Traveling Lecturer (APS, 1994-96); Max Planck Inst. Res. Award (1996); Chancellor's Prof. Berkeley (1997-2000); DOE Materials Sci. Award (1997); D.Sc. Honoris Causa, Hong Kong Univ. of Sci. and Tech. (1997) and Nat'l. Chao Tung Univ., (1998); Isakson Prize (APS, 1998); Member Nat'l Acad. Sci. (1995)., Amer. Acad. of Arts and Sci.(1990), Acad. Sinica (1990), Foreign Member, Chinese Acad. of Sci. (1996); Hon. Chair Prof. Nat'l. Tsing Hua Univ. (2001-07).

Personnel Commitments for FY2006 to Nearest +/- 10%:.D. Chemla (P.I.) 10%, R. Kaindl (Staff. Sci) 100%, J. Wang (Postdoc) 100%, I. Cotoros (GSRA) 35%, K. Dani (GSRA) 100%; J. Orenstein (P.I.) 30%, M. Langer (GSRA) 100%, C. Kantner (GSRA) 50 %; R. Schoenlein (P.I.) 70%, M. Rini Postdoc (100%); Y.R. Shen, (PI) 50%, J.McGuire (GSRA) 50%; Ji Na (GSRA) 50%, L. Zhang (GSRA) 50%.

Authorized Budget (BA):

FY04 $1390K	FY05 $1428K	FY06 $1307K

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020202

FWP and possible subtask under FWP: Synthesis and advanced characterization of nanoscale magnetic materials
D.T. Attwood, C.S. Fadley, P. J. Fischer, F. Hellman, J.B. Kortright

FWP Number: KC2204

Program Scope:
Novel magnetic nanoscale structures are synthesized and characterized with advanced techniques. The systems studied include vapor-phase deposited thin films and multilayers, structured or self-assembled nanoscale systems, nanoparticles, amorphous materials, metastable alloys, complex oxides, ferroelectric and multiferroic films, and nanocrystalline and single-crystal materials relevant to applications in spintronics and magnetics. Properties of interest include exchange bias; giant-, tunnel- and colossal- magnetoresistance; half-metallic ferromagnetism; and current-induced phenomena. Nano-calorimetric measurements yield electron, phonon, and magnon densities of states, as well as magnetic ordering temperatures. Advanced synchrotron-radiation techniques yield element-specific electronic and magnetic structures, including spatial resolution from micron to sub-nanometer scale, as well as time resolution to the picosecond scale. The methods include resonant soft x-ray scattering, soft x-ray microscopy, and high resolution spectroscopies (core- and valence- photoelectron, x-ray absorption, x-ray emission and inelastic scattering) excited by standing waves.

Major Program Achievements (This recently established group combines four established thrust areas)**:**

Synthesis and Calorimetry (Hellman):
- Significant improvements in micro/nanocalorimetry devices.
- Determination of thermodynamic properties of thin-film amorphous Si and Si-N.
- Development of a cluster model for perpendicular anisotropy in CoPt3 films.

Resonant soft x-ray scattering (Kortright):
- New insight into exchange-bias mechanism from depth-resolved magnetic reflectivity.
- Resolution of dipolar and exchange interaction effects in heterogeneous films and nanoparticle assemblies.
- Demonstration of molecular bond specific scattering at carbon *K* edge in heterogeneous polymer films.

Soft x-ray microscopy (Attwood, Fischer):
- Demonstrattion of 15 nm resolution in magnetization reversal studies of nanogranular CoCrPt alloy films.
- Development of stroboscopic pump-probe technique to study local spin dynamics with 70ps time resolution.
- Development of novel Fourier lenses for magnetic phase contrast imaging.

Soft x-ray spectroscopy (Fadley):
- Standing wave excited depth-resolved studies of electron and x-ray signals in GMR and MTJ systems.
- Observation of high-T electron localization in LSMO using multiple soft x-ray spectroscopies.
- Study of the oxidation at Si surfaces at multitorr pressures with time-resolved photoemission.

Program impact:
Development of new nanocalorimetric, soft x-ray scattering, soft x-ray microscopic and X-ray optics, and standing-wave spectroscopic techniques, and application of them to novel magnetic materials and nanostructures

Interactions:
A. Navrotsky (UCD)-calorimetry; D. Smith (ASU)-high-res. TEM, J. Mitchell (ANL)-oxide samples; R. Ramesh and Y. Suzuki (UCB), S.S.P. Parkin (IBM Almaden), E. Fullerton and I. Schuller (UCSD), K. Liu (UCD)-magnetic nanostructures; A. Epstein (OSU)-molecular magnets; H. Ade (NC State)-polymers; G. Meier (U Hamburg)-spin torque/transport; D. Allwood (Sheffield)-spintronic logic; G. Panacionne and F. Parmigiani (Trieste), C. Schneider (Jűlich), W. Wurth (U. Hamburg)-synchrotron radiation spectroscopy

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask): Hellman--APS Keithley Instrumentation Award; Fadley--Helmholtz-Humboldt Research Award (‘06)

Personnel Commitments for FY2007 to Nearest +/- 10%:
C.S. Fadley (50%)

Authorized Budget (BA:

FY04 $2361K	FY05 $2458K	FY06 $2150K

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020202

FWP and possible subtask under FWP: A Synergistic Approach to New Hydrogen Storage Materials, Part II
FWP Number: KC2205

Program Scope: This research is intended to generate new types of hydrogen storage materials with the potential for meeting the criteria required for making hydrogen fuel cell-powered vehicles feasible. In particular, nanostructured materials, such as boron nitride nanotubes and metal nanocrystal arrays, with the potential for attaining a reversible uptake of 6 wt % H_2 while operating at moderate temperatures and pressures are sought. A coordinated theory effort is in place to guide the experiments.

Major Program Achievements (over duration of support):
A Sieverts apparatus for the volumetric measurement of H_2 adsorption isotherms has been purchased, installed, and tested.

Both CVD and induction furnace methods have been refined for the large scale synthesis of pure BN nanotubes.

Conditions for varying the morphology of nanostructured BN have been identified. Testing of hyrdogen storage properties is underway to compare the effects of different morphologies.

CVD methods have been developed for the generation of composites of BN nanoparticles and metal or metal oxide nanoparticles.

Computational efforts have demonstrated a higher H_2 binding affinity for BN nanotubes compared to carbon nanotubes. In addition, the role of defect structures in enhancing H_2 binding has been explored.

A method has been developed for generating three-dimensional arrays of Pd nanocrystals with variation in diameter. Means of characterizing the hydrogen storage properties of such nanocrystal arrays have been devised.

Program Impact: The synthesis and characterization methods developed in the course of this program will be of value to other investigators in the field. Moreover, the new materials produced may ultimately serve as components of hydrogen storage systems for hydrogen fuel-cell powered vehicles.

Interactions: Close ties are maintained with the principle investigators and coworkers involved in Part I of this program (Jean Fréchet, Martin Head-Gordon, Jeffrey Long, and Thomas Richardson)
Sandia National Laboratory, Hydrogen Storage Program (Lennie Klebanoff, director)

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Alivisatos: ~30 plenary and invited lectures last year, including seven endowed lectureships; NSF Presidential Young Investigator, Sloan Foundation Fellow, Exxon, ACS Solid State Chemistry Fellowship, MRS Outstanding Young Investigator, Wilson Prize, Harvard, Fellow APS, Fellow AAAS, Visiting Professor St. John's College Cambridge, Colloid and Surface Chemistry ACS Award, elected to the National Academy of Sciences and the American Academy of Arts and Sciences, Larry and Diane Bock Chair in Nanotechnology, University of Chicago Distinguished Alumni Award, Rank Prize for Optoelectronics Award. *M. L. Cohen* – Fellow of APS; member of National Academy of Sciences; Sloan Fellow; Guggenheim Fellow; APS Buckley Prize; DOE Outstanding Accomplishment in Solid State Physics Award; DOE Sustained Outstanding Accomplishment in Solid State Physics Award; APS Lilienfeld Prize; U.S. National Medal of Science; ISI's top 100 most-cited physicists; President of the American Physical Society; member of American Philosophical Society; Foresight Institute Richard P. Feynman Prize in Nanotechnology; Harvard University Loeb Lecturer; University of Montreal Doctorat Honoris Causa; 50 invited talks since 2004. *S. G. Louie* – Fellow of APS; member of National Academy of Sciences; Sloan Fellow; Guggenheim Fellow; DOE Sustained Outstanding Research in Solid State Physics Award; APS Aneesur Rahman Prize; APS Davisson-Germer Prize; ISI's top 100 most-cited physicists; Foresight Institute Richard P. Feynman Prize in Nanotechnology; Outstanding Overseas Chinese Award; University of Chicago Closs Lecturer; Fellow of American Association for the Advancement of Science; 55 invited talks since 2004. *Zettl*: LBNL Outstanding Performance Award 2004, R&D 100 Award 2004, over 33 invited talks since 2003

Personnel Commitments for FY2006 to Nearest +/-10%: Rachel Smith (post-doc) 100%, Toby Sainsbury (post-doc) 100%
Authorized Budget (BA):
FY04 $0K **FY05** $535K **FY06** $535K

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020202

FWP and possible subtask under FWP: Experimental and Theoretical Investigations of Spin Transport
FWP Number: KC2206
Program Scope:
Conventional microelectronic devices are based on the ability to store and control the flow of electronic charge. However, the increasing amounts of power required by modern CMOS-based logic and memory devices is now a critical problem. Spin-based electronics promises a radical alternative, offering the possibility of logic operations with lower power consumption than equivalent charge-based logic operations. Our research team has the necessary experimental and theoretical skills to conduct research into the fundamental physics in support of a spin-based technology. Through collaboration with Prof. David Awschalom at UCSB, we have the ability to design and fabricate quantum well structures with tuned spin-orbit interactions. At LBNL, we have developed the transient spin grating technique for direct measurement of spin current. Finally, these capabilities are linked with a strong theoretical team at Stanford, led by Prof. Zhang.

Major Program Achievements (over duration of support):
Despite the fact that this is a new program, we have already seen major achievements.
Spin-Couomb drag: We have definitively observed a frictional force that opposes spin current in semiconductors. This force, known as "spin-Coulomb drag," had been theoretically predicted but not previously observed because of inability to quantitatively probe spin-diffusion coefficients. The existence of this frictional force, which acts specifically on spin current and not charge current, must be considered in the design of any spin current based device. **Persistent spin helix (theory):** We have investigated the spin dynamics that arise in a two-dimensional electron gas in the presence of both Rashba and Dresselhaus terms in the spin-orbit Hamiltonian. We have shown that an exact SU(2) symmetry arises when these terms are equal, leading to extremely long spin coherence times for certain spin helical states. **Persistent spin helix (experiment):** We have directly observed, using the spin transient grating technique, the enhanced lifetime of a spin helix state that arises when Rashba and Dresselhaus interactions coexist in the two-dimensional electron gas.

Program impact:
Spin-based electronics promises a radical alternative to charge-based logic operations, offering the possibility of logic operations with much lower power consumption. Our recent theoretical work suggests that spin transport is fundamentally different from the transport of charge. Ohm's law describes the inevitable dissipation of power in charge-current based devices. However, the generalized Ohm's law that governs the flow of spins indicates that the generation of spin current by an electric field can be less dissipative. To exploit the energy-saving potential of spin currents it is essential to be able to control them, as we control the flow of charge. Historically, spins have been manipulated by magnetic fields, which are difficult to control on the nanoscale. Recently it has been recognized theoretically that through spin-orbit coupling it is possible to manipulate spin currents *via* electric fields . In contrast to magnetic fields, nanoscale control of electric fields forms the basis of current integrated circuit technology and is therefore very highly developed. Electric-field control of spin, *via* spin-orbit coupling, will provide a far easier path to adopt spin-based devices into the mainstream of technology.

Interactions: Stanford University (Prof. S. Zhang); UC Santa Barbara (Prof. David Awschalom)

Recognitions, Honors and Awards Chair, Gordon Conference on Correlated Electron System (2002-2004) International and national invited talks, including APS March Meeting, Aspen Center for Physics, Institute for Theoretical Physics (Santa Barbara), International Center of Physics (Trieste), Gordon Conference on Superconductivity (Oxford, UK), and Symposium on SPC Coupled Materials (Tokyo).

Personnel Commitments for FY2003 to Nearest +/- 10%: J. **Orenstein** (group leader) 30%, Jacob Koralek (postdoc) 100 %

Authorized Budget (BA):
FY04 $0K **FY05** $0K **FY06** $122K

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020202

FWP and possible subtask under FWP: Novel sp^2-bonded Materials
FWP Number: KC2207

Program Scope:
Ab-initio quantum mechanical calculations to predict new materials structures and relate them to electronic structure and mechanical and thermal properties. Experimental synthesis of novel sp2-bonded materials including functionalized nanostructures, and characterization using SEM, TEM, STM, AFM, XRD, mechanical properties, and transport properties. Nanoscale device fabrication and testing. Strong connection between theory and experiment.

Major Program Achievements:
Theoretical prediction of new nanostructures including nanotubes and nanoparticles containing carbon, boron, and nitrogen. Theoretical analysis of nanparticles and hybrid structures and devices, including optical properties. Tuning of the bandgap of BN nanotubes and doping of carbon nanotubes studied theoretically and experimentally. Thermopower and thermal conductivity of nanotubes and nonlinear conductance of nanotubes determined theoretically. Nanobearings fabricated from nanotubes and frictional properties determined. Young's modulus of carbon and BN nanotubes determined. Electron holography of field-emitting nanotube performed. Oxygen sensitivity of nanotubes discovered. New fullerene-like materials synthesized. High resolution, low temperature UHV STM studies of BN nanotubes and carbon nanotube junctions and fullerenes performed. Zone-refinement of carbon nanotubes. High resolution STM studies of nanotubes and fullerenes.

Program impact:
Experimental demonstration of nanotube electronic device and nanotube nanobearing. Demonstration of nanotube sensitivity to environmental agents. Exciton behavior examined in semiconducting and metallic nanosystems. Discovery of BN nanotubes, silocrystals and nanoparticles. STM studies of BN nanotubes. Experimental verification of Giant Stark Effect in BN nanotubes. Controlled charge state of individual C60 molecule through reversible single-atom doping. Mapping of electronic structure of fullerenes and phase diagram of doped C60 molecular layers.

Interactions:
Internal: National Center for Electron Microscopy, National Scientific Computing Center (NERSC), Advanced Light Source, Berkeley Microfabrication Laboratory
External: University of Vienna, Max Planck Institute Stuttgart, University of Pennsylvania, Pennsylvania State University, UCLA, SUNY Stony Brook, Seoul National University, Korea, Hong Kong University of Science & Technology, and Universidad del Pais Vasco, Spain

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Alex Zettl – LBNL Outstanding Performance Award 2004, R&D 100 Award 2004, 33 invited talks since 2003.
C. Bertozzi - Elected to the National Academy of Sciences in May 2005, 91 invited talks since 2003.
M. L. Cohen –U.S. National Medal of Science; ISI's top 100 most-cited physicists; President of the American Physical Society; member of American Philosophical Society; Foresight Institute Richard P. Feynman Prize in Nanotechnology; Harvard University Loeb Lecturer; University of Montreal Doctorat Honoris Causa; 43 invited talks since 2003.
S. G. Louie –APS Davisson-Germer Prize; ISI's top 100 most-cited physicists; Foresight Institute Richard P. Feynman Prize in Nanotechnology; Outstanding Overseas Chinese Award; member of National Academy of Sciences; 48 invited talks since 2003.
M. Crommie – 10 invited talks since 2003.

Personnel Commitments for FY2006 to Nearest +/- 10%:
PI's (Zettl 25%, Bertozzi 10%, Cohen 25%, Louie 20%); Visiting Scientist: (Capaz, - fellowship 50%); Post Docs (Son 75%, Kirakosian 100%, Wiachwiak 100%, Kis 100%, Ikuno 50%, Regan 20%,); GSR's (Khoo 50%, Luo 50%, Fennimore 50%, Mickelson 50%, Begtrup 25%, Yuzvinsky 25%, Chang 25%, Jensen 25%, Girit 25%, Kessler 25%, Huang 25%, Comstock 50%, Chen 50%)

Authorized Budget (BA):
FY04 $1525K FY05 $1254K FY06 $1050K

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020203

FWP and possible subtask under FWP: Quantum Theory of Materials
FWP Number: KC2301

Program Scope: The emphasis of our research is on carrying out quantum-mechanical calculations for realistic systems based on microscopic first-principles approaches. Model systems are also examined, and new theoretical techniques are developed. Studies include bulk materials, fullerenes, nanotubes, graphene, superconductors, surfaces, materials under high pressure, two-dimensional electron systems, polymers, clusters, and defects in solids. Close collaboration with experimentalists is maintained. In addition, our program has a new component on strongly correlated systems. This involves developing phenomenological models for phenomena in complex oxides, exact solution of strong correlated models, and exploring physics beyond the Landau paradigm. Strong interaction with experiments will also be maintained.

Major Program Achievements (over duration of support): Explained properties of materials (e.g., bonding and structural properties; band structure and optical properties; properties of defects, surfaces, clusters and nanostructures) and predicted new materials and phenomena (e.g., superhard materials, new class of nanotubes, new phases of materials under high pressures, new superconductors). Developed new theoretical and computational methods. In strongly correlated physics, we have developed, by now, the standard model for describing STM data of high T_c superconductors. In addition, we have unified the existing mechanisms for charge fractionalization in condensed matter physics.

Program Impact: Led to discoveries of new materials and properties, explanation of experiments, and development of theoretical methods. Unification of charge fractionalization in polyacetylene and fractional quantum Hall effect is of such fundamental importance that its future impact is inevitable.

Interactions: Internal—NERSC/LBNL (Canning, Meza, Wang), MSD/LBNL (Chrzan, Crommie, Lanzari, Morris, Zettl), CSD/LBNL (Fleming, Head-Gordon); Molecular Foundry/LBNL; Advance Light Source, LBNL; UC Berkeley Center for Integrated Nanomechanical Systems; External—Yale, Harvard, Cornell, U of Washington, Palo Alto Research Center, LLNL, Georgia Tech, Penn State, U of Texas at Austin; International—Tokyo Institute of Technology (Japan), Seoul National University (South Korea), Korea Advanced Institute of Science (South Korea), Taiwan National Center for Theoretical Science (Taiwan), IU. Pais Vasco (UPV/EHU, Spain), KITP (Beijing, China), Fudan Univeristy (China); Center for Advanced Study (Tsinghua University, China).

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
M. L. Cohen – Fellow of APS; member of National Academy of Sciences; Sloan Fellow; Guggenheim Fellow; APS Buckley Prize; DOE Outstanding Accomplishment in Solid State Physics Award; DOE Sustained Outstanding Accomplishment in Solid State Physics Award; APS Lilienfeld Prize; U.S. National Medal of Science; ISI's top 100 most-cited physicists; President of the American Physical Society; member of American Philosophical Society; Foresight Institute Richard P. Feynman Prize in Nanotechnology; Harvard University Loeb Lecturer; University of Montreal Doctorat Honoris Causa; 50 invited talks since 2004. **D.-H. Lee** – Fellow of APS; Cheung-Kong Chair Professor, Center for Advanced Study, Tsinghua University, Beijing, China. **S. G. Louie** – Fellow of APS; member of National Academy of Sciences; Sloan Fellow; Guggenheim Fellow; DOE Sustained Outstanding Research in Solid State Physics Award; APS Aneesur Rahman Prize; APS Davisson-Germer Prize; ISI's top 100 most-cited physicists; Foresight Institute Richard P. Feynman Prize in Nanotechnology; Outstanding Overseas Chinese Award; University of Chicago Closs Lecturer; Fellow of American Association for the Advancement of Science; 55 invited talks since 2004.

Personnel Commitments for FY2006 to Nearest +/- 10%:
Principal Investigators (Cohen 30%, Lee 80%; Louie 20%); Post Doctorals (F. Giustino 100%; A. Seidel 100%; T. Ribeiro 25%); Grad students (J. Noffsinger 50%; D. Strubbe 50%).

Authorized Budget (BA):
FY04 $315K FY05 $315K FY06 $334K

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020203

FWP and/or subtask Title under FWP:
Predicting the Electronic Properties of 3D, Million-Atom Semiconductor Nanostructure Architectures

FWP Number: KC2302

Program Scope: To develop new computational approaches for thousand atom nanostructure calculations. Especially to develop the charge patching method, so the electronic structures and optical properties of thousand atom nanocrystals can be calculated with ab initio accuracy, replacing the empirical pseudopotential method, also to calculate the electronic structures of multicomponent nanostructure architectures.

Major Program Achievements (over duration of 2004-2005):
Mn impurity in a ZnS/ZnO core shell quantum dot: the Mn impurity level in valence band is above the valence band maximum (VBM) of ZnS, while the VBM of ZnO is also higher than the VBM of ZnS. By placing one Mn impurity at the center of ZnS core, we can couple the Mn impurity level with the ZnO VBM. This coupling can be controlled by the size of ZnS core, and the thickness of ZnO. More interestingly, this coupling can be modified by an applied electric field. Since Mn impurity level is magnetic (with only one spin), this type of system might have potential application in the optical-spintronic applications. We have used our charge patching method to study this system.

Magnetic field in the Pescan code: we have implemented the magnetic field effects in our Pescan code which uses the folded spectrum method to calculate the band edge states in a nanosystem. Now, our program includes all the relevant effects in a magnetic system: magnetic field, spinor electron wavefunction, spin-orbit couping. One application of these capabilities is to study the magnetic moment precession under an electric field (the g-factor), and ultra-fast dynamics of the many body wavefunctions after pulse optical stimulation in a quantum dot. This can be done by combining the Pescan calculaton with the limited CI calculation for exciton energies. We are at the initial stage of studying these phenomena.

ZnO/ZnTe, ZnO/ZnS optical spectra: ZnO, ZnS are environmentally benign materials with relatively large optical band gaps (~3.5 eV). To use them for solar cell related applications, we need to make their band gap close to 1 eV. One idea is to have heterostructures of ZnO/ZnS, or ZnO/ZnTe. Due to their type-II band alignment, the overall band gap should be much smaller, and the optical oscillator strength should be appreciable if the individual layer of each material is not thick. We have used our charge patching method, combined with a correction for the LDA band gap to calculate the optical spectra of such systems: both for superlattices and core/shell quantum wires. For ZnO/ZnTe the band gap is around 1.3 eV, but for ZnO/ZnS the band gap is around 2 eV.

CdTe tetrapod under load: In collaboration with an experiment in LBNL, we have calculated the shape deformation of a CdTe tetrapod when it is placed on a substrate and the top of the tetrapod is pressed by an applied load via the AFM tip. This is calculated using a valence force field model. The deformed tetrapod is calculated for its electronic structures using the semi-empirical pseudopotential method. Our calculation helps to explain the experimental results..

Charged dopant level: While we have calculated many charge neutral isoelectronic impurity levels, it is still a challenge to calculate the charged dopant level. The dopant levels have been studied via the k.p model forty years ago, but the chemical potential near the impurity is not known. Thus, the absolute impurity level binding energies have never been predicted quantitatively. We have started to investigate this using our charge patching method and our polarization motifs.

Program Impact:
The development of the charge patching method enables us to calculate thousand atom nanosystems with ab initio accuracy. The calculation is fast and scales linearly to the size of the system.

Interactions:
National Renewable Energy Lab: (A. Zunger). Univ. of Tennessee: (Jack. J. Dongarra).

Personnel Commitments for FY2004 to Nearest +/-10%:
Lin-Wang Wang 15%
Joshua Schrier (post-doc) 100%
Authorized Budget (BA):
FY04 $175K FY05 $165K FY06 $165K

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020203

FWP and/or subtask Title under FWP:
Charge patching method for electronic structures and charge transports of organic and organic/inorganic mixed nanostructures

FWP Number: KC2303

Program Scope: (1) extend and test the charge patching method (CPM) to organic molecules, generate the ab initio electron charge density of these organic molecules without doing direct ab initio calculations; (2) use the folded spectrum method and the single particle Hamiltonian from the patched charge density to study the electronic properties of thousand atom inorganic/organic mixed systems; (3) use CPM in the force field model for the nonbonding interactions for total energy calculations, and develop linear scaling electronic structure calculation methods for organic and organic/inorganic mixed nanostructures.

Major Program Achievements (over duration of 2006 Sept.-2006 Dec.):
This project is funded around Sept. 2006. So it is still at its beginning stage. We are still in the process of hiring postdoctoral fellows for this project.

The charge density of alkane chain (C_nH_{2n+2}): We are using the CPM to calculate the charge density of alkane chain, and compare the results and the subsequent electronic structures with the direct local density approximation (LDA) results. The key in this investigation is to study the dependence of the charge density on the -CH_2-CH_2- torsion angle, and whether a same charge density motif can be used for different torsion angles. We are only at the initial stage of this project.

Linear scaling 3 dimensional fragment method (LS3DF): We have developed a linear scaling electronic structure calculation method for thousand atom inorganic nanocrystals and organic molecules. This is a selfconsistent total energy calculation method. The LS3DF divides the whole system into small overlapping fragments. It calculates the electronic structures of each fragment independently using a small group of computer processors, and then patches up the total charge density of the system using a novel patching scheme. This scheme assures that the artificial surface effects created by the division will be cancelled out among different fragments. As a result, the LS3DF yields almost the same result as the direct LDA calculation: the energy difference is about a few meV per atom, the charge density difference is about 0.2%, and the atomic force difference is about 10^{-5} a.u. These differences are smaller than the differences introduced by other numerical uncertainties (e.g, due to planewave basis truncations, and the use of pseudopotentials). Due to the independent solution of each fragment (no communication is needed), the code is easily parallelizable. Our code has been tested to scale well to one thousand processors, and it has been used to calculate a Si quantum dot containing 15,000 Si atoms.

Program Impact:
The development of the LS3DF method allows us to calculate >10,000 atom systems directly. It is a candidate for future petascale computing.

Interactions:

Personnel Commitments for FY2005 to Nearest +/-10%:
Lin-Wang Wang 15%
post-doc to be hired: 100%

Authorized Budget (BA):

FY04 $0K	FY05 $0K	FY06 $0K (FY07 $275K)

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020301

FWP and possible subtask under FWP: Mechanical and chemical properties of surfaces and interfaces
FWP Number: KC3101

Program Scope:
Fundamental studies of surface structure, friction, lubrication, wear. Energy transfer in nanometer contacts. Atomic scale manipulation. Development of advanced atomic scale imaging and spectroscopy techniques: Scanning Tunneling and Atomic Force Microscopies (STM and AFM), High Pressure Photoelectron Spectroscopy (HPPES).

Major Program Achievements (over duration of support):
-Nanotriboloby: Molecular scale friction mechanisms in lubricant monolayers. Determined molecular packing of alkyl-silanes, -amines and -alcohols (application to MEMS).
-Discovered enhancement of friction in Si pn junctions during forward bias of highly doped regions.
-Determined forces generated by dipole fields at atomic steps of metal surfaces.
-Determined velocity dependence of friction related to nature of hydrogen bonding in surface layers
-Molecular manipulation: Determination of mechanisms of excitation of vibrations, rotations, dissociation and translations of single atoms and molecules during tip-substrate interactions.
-Discovered effect of electric fields on binding energy of H on Pd surfaces leading to diffusion and dissolution.
-Structure of water on metals: partial dissociation of water on Ru(0001) surfaces upon annealing leads to mixed elongated islands of water and hydroxyl groups.
-Phase diagram of Pd oxidation determined *in situ* using photoelectron spectroscopy.
-Role of defects on TiO2 to form OH groups that act as nucleation centers for H2O growth studied by *in situ XPS.*
-Determined structure of Pt catalyst surface and nature of CO poisoning during H2-D2 exchange reaction *in situ* by STM and by XPS.
- Electronic cross-talk between Au nanoclusters due to proximity effects using mechanical compression. Electronic and ligand structure examined by photoelectron spectroscopy (XPS and NEXAFS).

Program impact:
Provide insights into mechanisms of energy dissipation in friction, lubricant monolayers under pressure (MEMS, Hard Disk lubes). Discovered unusual friction dependence on carrier density on Sip n junctions with potential for friction control in nanomachines. Enabled imaging of liquids with nanometer resolution (previously not possible). Enabled studies of catalysis and environmental science *in situ* using atomic resolution imaging and photoelectron spectroscopy.

Interactions:
Internal: Molecular Environmental Science project at ALS beam line 11. Surface Science and Catalysis (Gabor Somorjai). Molecular Foundry (Alivisatos, Frechet, Bokor, Louie, Bertozzi). External: AMES Laboratory: (tribology of quasicrystals). Sandia Natl. Lab. (Peter Feibelman, theory). Univ. Autonoma Madrid, Spain (STM theory). Ecole Normale Superieure Lyon, France (STM theory). Spanish National Research Council (tribology of monolayers). Univ. Barcelona, Spain: (organic monolayers, *ab-initio* calculations). Fritz-Haber-Institut Berlin, Germany: HPPES**.** University of Paris-VI: *ab-initio* calculations of chemisorption.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Keynote Speaker Royal Academy of Sciences. Sevilla, Spain. May 19, 2006. Keynote speaker at Closing Ceremony of the World Year of Physics. Parlament of Catalunya. Barcelona, Spain, December 14, 2005.

Personnel Commitments for FY2006 to Nearest +/- 10%:
Staff: M. Salmeron (20%), Postdocs: Frank Rose (100%), Sacha Gomez (25%). Students: Mousslim Tatarkhanov, Tomoko Shimizu, Yabing Qi, Ingeborg Stass (100%), Admin: Alice Muller-Egan (50%)

Authorized Budget (BA):

FY04 $435K	FY05 $421K	FY06 $405K

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020301

FWP and possible subtask under FWP: Surface Science and Applications Program
FWP Number: KC3102

Program Scope:
The structure and composition of solid surfaces (metal single crystals, nanoparticles and polymer thin films) and adsorbed monolayers are determined on the atomic scale with continually increasing spatial and time resolution. STM, AFM, and SFG techniques are utilized in most of these studies applied at high pressures and at liquid interfaces. The rate and selectivity of catalyzed surface reactions are studied using single crystal surfaces and nanoparticles, *in situ*, and correlated with surface structure and composition. Instruments have been built that permit molecular level surface studies from high pressures to ultra high vacuum, over fourteen orders of magnitude pressure range using SFG-surface vibrational spectroscopy, STM and AFM. Adsorption and surface structure of peptides are studied on hydrophobic and hydrophilic surfaces by SFG. For the first time, the atomic level surface properties can be studied during adsorption and during chemical reactions at high pressures and temperatures and at solid-liquid interfaces.

Major Program Achievements (over duration of support):
The high pressure, high temperature scanning tunneling microscope (STM) allowed in-situ examination of surfaces under catalytic conditions in real time and on the molecular scale. Organic molecules on the catalytically active platinum and rhodium surfaces are mobile. When the hydrogenation reaction is poisoned by the co-adsorption of CO the molecular motion is frozen and an ordered adsorbate layer forms. Surface mobility of molecules and catalytic activity is correlated. SFG studies show that CO dissociation is surface structure sensitive when it occurs on platinum single crystal surfaces. The temperature where CO dissociation occurs coincides with the ignition of CO oxidation. This finding implicates CO dissociation as the primary cause of the ignition of combustion. Reaction intermediates are detected by SFG during hydrocarbon conversion at high pressures on metal single crystal and monodispersed nanoparticle (Pt, Rh) surfaces. Adsorption of peptides reveals changes of structure and composition on hydrophobic and hydrophilic interfaces in water solution utilizing SFG.

Program impact:
Determined the molecular ingredients of surface chemical reactivity; the mobility of surface atoms and molecules, and the metal surface structure. Changes of bonding of peptides on hydrophobic and hydrophilic surfaces was detected.

Interactions:.
Polymer Technology Group, Berkeley CA; Qualcom, Inc., San Jose, CA; Intel Corp., Santa Clara, CA; University of California, Berkeley: Prof. Jeff Bokor, Electrical Engineering; Prof. Kyriakos Komvopoulos, Mechanical Engineering; Prof. Song Li, Bioengineering and Prof. Peidong Yang and Professor Paul Alivisatos, Chemistry.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
2007, Langmuir Prize; 2006, Remsen Award from the Maryland Section of the ACS; Honorary Fellow, Cardiff University; 2003, Cotton Medal, Texas A&M University.
30 invited talks since January 2005

Personnel Commitments for FY2004 to Nearest +/- 10%: Gabor **Somorjai** (PI) 20%
Miguel Salmeron (Sr. Staff Scientist) 20%; Feng Tao (post-doc) 100%; Jeong Park (post-doc) 80%;; Katie Bratlie, Saskia Kweskin, Roger York, Derek Butcher, Chris Kliewer and George Holinga (students) 50%

Authorized Budget (BA):

FY04 $740K	FY05 $740K	FY06 $740K

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020301

FWP and possible subtask under FWP: Microscopy Investigations of Quantum Dots, Nanorods, and Soft Condensed Matter
FWP Number: KC3103

Program Scope:
This program aims to stretch the limits in the state-of-the-art of optical characterization, through the development of novel forms of optical microscopies, such as single pulse CARS microscopy with phase control, apertureless NSOM (ANSOM), and femtosecond pump-optical injection probing spectroscopies of single nanostructure species under stimulated emission conditions. A parallel molecular beam epitaxy growth effort for processing semiconductor materials with in situ scanning tunneling microscopy is used to study the growth mechanisms of III-V nitrides and doped nitrides. Development of novel microscopies provide new spectral and spatial windows into the analysis of materials for DOE missions in energy utilization.

Major Program Achievements (over duration of support):
Growth studies of flat GaN and InN, as well as islands of InN and InGaN have been performed in an apparatus that incorporates scanning tunneling microscopy with molecular beam epitaxy. Growth mechanisms of GaN have been analyzed by tunneling microscopy images. Apertureless near field microscopy studies of GaN and InN islands have revealed contrast mechanisms due to the real and imaginary parts of the index of refraction, measuring nanometer size Ga metal islands, and probing InGaN islands. Pickup of gold nanoparticles permits tip enhancements with resolution of the electric field phase in the images, as well as tests of the dipole model for tip radiators. Tips are being developed with pre-functionalized gold particles. Ultrafast laser, differential gain experiments on ZnO lasing in nanowires and tetrapods have been performed to measure the timescales and ratios of electron-hole plasma and exciton mechanisms during lasing in nanostructured materials. Using upconversion methods, the wavelength and time dependences of the lasing pulses from individual nanowires are measured for the first time. A single pulse CARS microscopy project using an ultrafast laser and phase control with interferometric detection produces complete Raman spectra while spatially scanning. Polymer domains have been analyzed with vibrational spectral sensitivity, and new work is addressing bacterial spores and multilamellar membranes.

Program Impact:
New forms of microscopy with chemical specificity have significant impact on the semiconductor industry, related to the study of patterning, line dimension reduction, nanostructure lasers, and materials analysis. Studies of InGaN and alloyed nitrides are important for the lighting industry and for solar conversion efficiency.

Interactions:
A collaboration with ALS and Molecular Foundry scientists involves the study of polymer cross linking.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
Invited Speaker at American Chemical Society Somorjai symposium. Invited speaker at American Physical Society March Meeting.

Personnel Commitments for FY2005 to Nearest +/- 10%:
S. **Leone** (PI) 5%, A. Tivanski (postdoc) 20%, G. Dengel (visiting student) 80%, A. Caster (graduate student) 10%, J.-K. Song (postdoc) 70%, S.-H. Lim (postdoc) 10%, Olivier Nicolet (postdoc) 10%, Larissa Stebounova (postdoc) 80%, S. Baer (postdoc) 10%

Authorized Budget (BA):
FY04 $390K FY05 $390K FY06 $390K

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020301

FWP and possible subtask under FWP Self-assembly of organic/inorganic nanocomposites materials
FWP #: KC3104
Program Scope: Create functional materials by parallel and hierarchical self-assembly. Develop wet chemical processes by which organic/inorganic composites can be created with a high degree of control on many length scales simultaneously. By developing a comprehensive ability to pattern organic/inorganic composites, it will be possible to design complex materials in which several microscopic processes are independently and simultaneously optimized. Target functional materials with applications in energy conversion, mechanical composites, and optical/electrical devices. The team: Paul Alivisatos (inorganic nanocrystals); Jean Frechet (Polymers and Organic Synthesis); Miquel Salmeron (Spectromicroscopy) ; Lin Wang Wang (Theory); Daniel Chemla (spectroscopy) .
Major Program Achievements (over duration of support): Demonstrated the concept of hybrid inorganic-organic nanorod – polymer solar cells (Science 2002, *295*, 2425.); developed dual nanocrystal solar cell (Science 2005); General route to vertical ZnO nanowire arrays using textured ZnO seeds (Nano Lett 2005); Nanowire dye-sensitized solar cells (Nature Materials, 2005); developed new specialty electro-active surfactants that solubilize inorganic nanorods, while permitting electron transfer (Adv. Mat. 2002); calculated the energy levels of semiconductor nanorods vs. aspect ratio, and verified the prediction that the degree of polarization should change dramatically at aspect ratio of 2 (Science 2001, *293*, 1455, Journal of Physical Chemistry B 2002, *106*, 2447); discovered the existence of liquid crystal phases of inorganic semiconductor nanorods (Nano Letters 2002, *2*, 557.). Computed the energy levels of exotically shaped nanocrystals – arrows and teardrops (Nano Letters 2003); demonstrated the synthesis in high yield of branched nanocrystals(Nature materials 2003) and hyper-branched nanocrystals (Nano Letters, 2005); demonstrated the growth of nanocrystals by microfluidic techniques (Nano letters 2003, JACS 2005); demonstrated solution phase X-ray absorption spectroscopy of Co nanocrystals; Electrical and AFM investigations of individual inorganic tetrapods.
Program Impact: Examples of Applications: hybrid nanorod – polymer solar cells; light emitting diodes; mechanical reinforcement of plastics. Education: About 300 scientists have been trained in the combined labs, and are now active in the science community. (alumni at Arkansas, Cambridge University, Bain Consulting, Exxon-Mobil, General Electric, Univ. of Hamburg, Harvard, Hebrew Univ. of Jerusalem, Intel, Univ. of Mainz, MIT Media Lab, Mitsubishi Chemical, Nanosys, Covio, Naval Research Lab, Patent Attorney, Quantum Dot Corp., Rice, National Taiwan University, Siemens, UCLA, Vanderbilt). Patents: Ten issued. Founded two companies: Quantum Dot Corporation (fifty employees) with focus on biomedical applications of semiconductor nanocrystals, and most recently, Nanosys, with focus on electro-optic applications. Press Articles: C&E News, Science, Nature, Science News, Scientific American, MIT Technology Review, Red Herring, Business Week Service to the community: Founding editor-in-chief of Nano Letters (American Chemical Society); **Interactions:** Current team members: Paul Alivisatos (Chemistry and MSD) Jean Frechet (Chemistry and MSD), Miquel Salmeron (MSD); LinWang Wang (NERSC); Collaborators: Richard Mathies (Chemistry) (Daniel Chemla (Physics and MSD), Alex Pines (MSD and Chemistry), Anupam Mahukar (USC), Ned Seeman (NYU), Laura Landweber (Princeton), Priya Vashista (LSU), Lydia Sohn (Princeton). Former collaborators: Chuck Shank, Peter Schultz, Paul McEuen. Industry Interactions: 3M, Dow Chemical, Dupont, Intel, Kodak, Motorola, Xerox; Bayer, BASF, Mitsubishi Chemical, Samsung.
Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask): Alivisatos: ~30 plenary and invited lectures last year, including seven endowed lectureships; NSF Presidential Young Investigator, Sloan Foundation Fellow, Exxon, ACS Solid State Chemistry Fellowship, MRS Outstanding Young Investigator, Wilson Prize, Harvard, Fellow APS, Fellow AAAS, Visiting Professor St. John's College Cambridge, Colloid and Surface Chemistry ACS Award, elected to the National Academy of Sciences and the American Academy of Arts and Sciences, Larry and Diane Bock Chair in Nanotechnology, University of Chicago Distinguished Alumni Award, Rank Prize for Optoelectronics Award. Fréchet: NAS, NAE, AAAS; ACS Award n Polymer Chemistry, Butler Lecturer Florida, ACS Salute to Excellence Award, ACS Cope Scholar Award, Baker Lecturer Cornell, Stauffer Lecturer Stanford, Bayer Lecturer, Pittsburgh, Chute Lecturer Dalhousie, Merk-Frosst Lecturer Alberta, Chambers Lecturer Rochester, Dow Karabatos Lecturer Michigan State, Doctorate (Honoris Causa) Universite Claude Bernard, France. Salmeron: Plenary lecturer 18th European Conf. on Surface Science, Keynote speaker 1st Latin American Sym. on Scanning Probe Microscopy. 13 invited talks since 2001. Yang: 2005, ACS Pure Chemistry Award
Personnel Commitments for FY2003 to Nearest +/-10%: P. **Alivisatos** (PI), M. Salmeron (senior scientist) 10%, D.F. Ogletree (staff scientist) 10%, 12 100% graduate students, 8 100% postdoctoral fellows, 2 visitors.
Authorized Budget (BA):
FY04 \$1359K **FY05** \$1228K **FY06** \$1253K

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020301

FWP and possible subtask under FWP: Physical Chemistry of Nanocrystals
FWP Number: KC3105
Program Scope: Nanometer size inorganic crystals are playing an increasingly important role in solid-state physics, chemistry, materials science, and even biology. Many fundamental properties of a crystal (e.g., ionization potential, melting point, band gap, saturation magnetization) depend upon the solid being periodic over a particular length scale, typically in the nm regime. By precisely controlling the size and surface of a nanocrystal, its properties can be tuned. Using techniques of molecular assembly, new nanocrystal-based materials can in turn be created. This program encompasses fundamental studies of the mechanisms and kinetics of nanocrystal synthesis as well as studies of scaling laws for optical, electrical, magnetic, and structural size dependent properties.
Major Program Achievements (over duration of support): Helped develop the concept of inorganic nanocrystals as a class of macromolecule. First studies of surface derivitization and isolation of nanocrystals, and immobilization of nanocrystals on self-assembled monolayers; first photoelectron spectroscopy studies of nanocrystal electronic structure (with Jim Tobin) and nanocrystal surface structure. X-ray Absorption Spectroscopy as a tool for determining nanocrystal surface structure; first measurements of single nanocrystal x-ray absorption spectra. Synthesis and shape control of semiconductor nanocrystals and nanorods of CdSe, InP, InAs, GaAs, Co, and Fe_2O_3. Discovery of branching in nanorod synthesis of II-VI semiconductors, including synthesis of tetrapods and inorganic dendrimers. Studies of core-shell nanocrystal synthesis and properties. Optical properties of nanocrystals, including hole-burning, resonance Raman, photon echo, Stark effect; polarization and blinking studies of quantum dots and nanorods. Studies of pressure and temperature induced structural transformations in nanocrystals. Single nucleation events in nanocrystal structural transformations; shape change as an indicator of mechanism in nanocrystal transformations, first measurements of activation energy and activation volume in nanocrystal structural transformations. Hollow nanocrystal formation through the nanoscale Kirkendall effect. Cation exchange kinetics, reversibility, mechanism in nanocrystals. First electrical device based on a nanocrystal-polymer composite (light emitting diode); first transistor based on a single nanocrystal and a single molecule (with Paul McEuen); developed the use of DNA as a tool for patterning nanocrystals (with Peter Schultz); discovered liquid crystal phases of semiconductor nanorods; introduced the use of colloidal quantum dots as fluorescent biological labels (with Shimon Weiss); first demonstrated the plasmon spectroscopic ruler for measuring nanoscale distances. Hybrid nanorod-polymer solar cell. Dual Nanocrystal Solar cell
Program impact: Light emitting diodes, solar cells, solar concentrators, fluorescent biological labels (reduced photobleaching, multiplexed assays), magnetic storage, magnetic bio-labeling, mechanical reinforcement of composites. Education: About 100 scientists have been trained in the lab, and are now active in the science community. (alumni at Arkansas, Bain Consulting, Cambridge University, Exxon-Mobil, General Electric, Univ. of Hamburg, Harvard, Hebrew Univ. of Jerusalem, Intel, Univ. of Mainz, MIT Media Lab, Mitsubishi Chemical, Nanotectonica, Nanosys, Naval Research Lab, Patent Attorney, Quantum Dot Corp., Rice, National Taiwan University, Siemens, Stanford, UCLA, Vanderbilt).
Interactions: Current collaborators: Jan Liphardt (Physics and PBD), Phil Geissler (Chemistry and PBD), Jean Frechet (Chemistry and MSD), Daniel Chemla (Physics and MSD), Alex Pines (MSD and Chemistry), Anupam Mahukar (USC), Ned Seeman (NYU), Priya Vashista (LSU), Wendell Lim (UCSF); Former collaborators: Chuck Shank, Peter Schultz, Paul McEuen. Industry Interactions: Founder, Quantum Dot Corporation; Founder, Nanosys, Inc.
Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask): Patents: Ten issued. Founded two companies: Quantum Dot Corp. (fifty five employees) with focus on biomedical applications of semiconductor nanocrystals, and most recently, Nanosys, with focus on electro-optic applications. Small Times 2003 Researcher of the Year. 2nd most cited scientist in nanotechnology for 1993-2003 (ISI). Press Articles**:** C&E News, Science, Nature, Science News, Scientific American, MIT Technology Review, Red Herring, Business Week, Service to the community: Founding editor, Nano Letters (ACS); Associate Editor, Ann. Rev. of Phys.Chem.; co-author with Mike Roco (NSF) and Stan Williams (HP) of the National Nanotechnology Initiative Report. DOE Council on Materials Science; External Review Board of the Joint Institute of Laboratory Astrophysics; National Research Council Solid State Sciences Subcommittee. Examples of Awards and Honors: ~30 plenary and invited lectures last year, including seven endowed lectureships; NSF PYI, Sloan Foundation Fellow, Exxon ACS Solid State Chemistry Fellowship, MRS Outstanding Young Investigator, Wilson Prize, Harvard Univ., Fellow, American Physical Society, Fellow, AACS, Visiting Professor St. John's College Cambridge, Colloid and Surface Chemistry ACS Award, member, Nat. Acad. of Sciences and the Am. Acad. of Arts and Sciences, Larry and Diane Bock Chair in Nanotechnology, Univ. of Chicago Distinguished Alumni Award, Rank Prize for Optoelectronics Award.
Personnel Commitments FY2006: A.P. **Alivisatos**-PI (10%), 4 100% graduate students, 2 100% postdoctoral, 1 50% postdoctoral, 1 16% postdoctoral visitors.
Authorized Budget (BA):
FY04 $415K **FY05** $615K **FY06** $615K

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020301

FWP and possible subtask under FWP: Multi-component assembly of high surface-area ordered oxide-metal nanocomposites with enhanced catalytic properties.
FWP Number: KC3106

Program Scope: Developing novel synthetic strategies for shape-controlled growth of Au, Pt and bimetallic nanocrystals, ideally with one type of surface exposed only; 2-dimensional assembly of these nanocrystals using Langmuir-Blodgett technique; 2- and 3-dimensional Assembly of these shaped nanocrystals within ordered porous oxide (SiO_2, Al_2O_3, TiO_2) matrix; Chemical reaction testing on the ordered metal-oxide nanocomposites to examine the effect of surface type of the nanocrystals, interface and surface area on the catalytic activity and selectivity.

Major Program Achievements (over duration of support):
(1). Cubic, cuboctahedral, and porous Pt nanoparticles were prepared using tetradecyltrimethylammonium bromide as a surface stabilizing reagent. The morphology was controlled by adjusting reduction methods. In-situ H_2 production from $NaBH_4$ enabled the synthesis of uniform nanoparticles. By changing the pH, which contributes to control of the reduction rate, shape evolution from cuboctahedra to cubes was observed. The nanoparticles which are electrostatically capped with alkylammonium ions and shape-controlled without aid of foreign metal ions show superior catalytic activity in comparison to nanoparticles prepared with a polymeric stabilizing reagent and silver. At 100^oC, C_{14}TABr-capped cubes were ~10 times more active than PVP-capped cubes. PVP-capped cuboctahedra prepared with 11mol% Ag showed no catalytic activity in the current reaction condition. C_{14}TABr-capped porous nanoparticles had the highest activity for ethylene hydrogenation due to much larger surface area comparing with cube or cuboctahedra.
(2). We discovered the spontaneous formation of ordered gold and silver nanoparticle stripe patterns upon dewetting a dilute film of polymer-coated nanoparticles floating on a water surface. Well-aligned stripe patterns with tunable orientation, thickness, and periodicity at the micrometer scale were obtained by transferring nanoparticles from a floating film onto a substrate in a dip-coating fashion. This facile technique opens up a new avenue for lithography-free patterning of nanoparticle arrays for various applications including for example multiplexed surface enhanced Raman substrates and templated fabrication of higher-order nanostructures.
(3). Monodisperse platinum nanoparticles with well-defined faceting have been synthesized by a modified polyol process with the addition of silver ions that control the platinum surface structure. Pt nanoparticles are encapsulated in mesoporous silica during *in-situ* hydrothermal growth of the high surface area support. Removal of the surface regulating polymer, poly(vinylpyrrolidone), was achieved using thermal oxidation-reduction treatments. Catalysts were active for ethylene hydrogenation after polymer removal. Rates for ethylene hydrogenation decreased in accordance with the amount of Ag retained in the Pt nanoparticles after purification. Ag is most likely present as small crystallites on the Pt particle surface.

Program Impact:
Enabling the deterministic assembly of high surface-area oxide-metal nanocomposites with enhanced catalytic activity and selectivity (i.e. catalyst-by-design).

Interactions:
G. Somorjai (Chemistry): Catalytic reaction studies on the high surface-area ordered metal-oxide nanocomposites.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):

2006	Molecular Science Forum Professorship, Institute of Chemistry, Chinese Academy of Science.
2006	Yangtze Scholar, Chinese Ministry of Education
2006	McElvain Lectureship, Department of Chemistry, University of Wisconsin, May, 2006.

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Personnel Commitments for FY2006 to Nearest +/-10%:
P.D. **Yang** (PI) 20%**;** H. Lee (postdoc) 100%; Susan Habas (graduate Student) 100%

Authorized Budget (BA):
FY04 $195K FY05 $195K FY06 $195K

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020301

FWP and possible subtask under FWP: Nuclear Magnetic Resonance
FWP Number: KC3107
Program Scope: The nuclear magnetic resonance (NMR) program has two complementary components. The first is the establishment of new concepts and techniques in NMR and its offspring, magnetic resonance imaging (MRI), in order to extend their applicability and enhance their capability to investigate molecular structure and organization from materials to organisms. The study and diagnostic use of nuclear spins interacting with each other and with others degrees of freedom requires the development of new theoretical and experimental methods; one consequence of these efforts is the design and fabrication of next-generation NMR and MRI equipment. The second component of the research program involves the application of such novel methods, together with other programs, and with outside laboratories and industry, to significant problems in chemistry, materials science, and biomedicine. It is the unique environment of interdisciplinary research and large-scale instrumentation capabilities at the Lawrence Berkeley National Laboratory that cultivates these innovations, their diverse applications, and technology transfer.

Major Program Achievements (over duration of support): Some principal developments: Helped launch high-resolution solid-state now widely used in materials, chemistry and biology; introduced multiple-quantum spectroscopy; developed zero-field Fourier-transform NMR using both field cycling and superconducting detectors; introduced dynamic-angle spinning and double rotation for quadrupolar nuclei such as oxygen-17 and aluminum-27; made advances in optically pumped and detected NMR and MRI, and the development of novel xenon and para-hydrogen-based highly polarized NMR molecular sensors; most recently, introduced ex-situ scanning, remote detection, and ultralow and zero-field SQUID and laser magnetometer detection of NMR and MRI, opening the way to in-the-field observation of objects and subjects not amenable to normal methods of NMR and MRI. Examples of applications: flow, mixing , and dispersion of fluids in porous materials, and recent development of microfluidic NMR and MRI "on a chip," studies of structure and dynamics in minerals and oil reserves, molecular assays, catalysts, semiconductors, surfaces, amorphous materials, quantum dots, polymers and dendrimers, biomolecules, biosensors, tissue, organisms, diagnostic biomedical molecular imaging.

Program impact: "Seeing is believing"; novel techniques and devices of magnetic resonance spectroscopy and imaging have expanded our ability to "see" into materials and organisms. The concepts and instrumentation, adopted worldwide by laboratories and industry, are being used to investigate molecular structure and organization from the nanoscale dimensions of catalysts and polymers to the macroscopic proportions of human imaging and oil exploration. Education: hundreds of scientists ("Pinenuts") trained in the laboratory, many holding leading positions in academia and industry. Patents: more than twenty issued, filed, pending or disclosed methodologies licensed, adapted into commercial NMR technology. Journal Covers and News Recognition: eg Nature, Nature Materials, Nature "News and Views", Science, Science "Perspectives", Technology Review, Photonics.com, New ScientistTech, Spectroscopy, J. Mag. Resonance, Angewandte Chemie, J. Physical Chemistry, C&E News, Science News, Biophotonics, Analytical Chemistry, R&D Magazine., PNAS "Commentary", Physics World.

Current Interactions: J. Reimer (EEHS and Chemical Engineering), D. Wemmer (Physical Biosciences and Chemistry), J. Clarke (MSD and Physics), D. Budker (NSD and Physics), T. Budinger and S. Conolly (LSD and Bioengineering), S. Prusiner and M. Shuman (UCSF). Industry: eg Schlumberger-Doll Research, GE, Varian.

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask): e.g. Glenn T. Seaborg Chair, UC Berkeley; Docteur Honoris Causa Universities of Rome and Paris: Member, National Academy of Sciences; DOE E.O. Lawrence Award; Wolf Prize in Chemistry; Centenary Medal, Royal Society of Chemistry; ACS Irving Langmuir Award; ACS F.A.Cotton Medal; Tetelman Fellow, Yale U; Ampere Congress Honoring AP's 50'th Birthday; R&D-100 Awards; Univ Calif Distinguished Teacher Award; Professeur Joliot-Curie; Ecole Superieure Phys Chem, Paris; Loeb Lecturer, Harvard U; Lord Lecturer, MIT; Roberts Lecturer, Caltech; Hinshelwood Professor, Oxford U; Lord Todd Professor, Cambridge U; Faraday Medal Royal Society; Seaborg Medal UCLA; Scientific American "50 Visionaries;" Elected Foreign Member, Royal Society (London): 60th Birthday International Ampere Symposium in Honor of Alex Pines, Chamonix France (2005); Medal of the NMR Society of Japan (2005); Distinguished Visiting Professor several Institutions (2006): new patents (2006)
Web Pages: http://waugh.cchem.berkeley.edu/research/ http://waugh.cchem.berkeley.edu/alex/

Personnel Commitments for FY2006: A. **Pines** PI 25%, 14 graduate students, 6 postdoctoral fellows.

Authorized Budget (BA):
FY04 $872K FY05 $872K FY06 $872K

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020301

FWP and possible subtask under FWP: Plastic Electronics
FWP Number: KC3108
Program Scope:
This program is aimed at the development of the fundamental understanding of the molecular and physical principles that govern the design of novel materials for organic or plastic electronics. The program aims at the exploration of newly designed materials, the determination of their physical and functional properties, and the comparison of these properties with those of known materials to provide access to a better understanding of the design rules and structure-property relationships for this important family of energy related materials. Based on novel design concepts the synthesis of new organic molecules, oligomers and polymers with interesting electrical and optical properties will be explored. The novel materials will then be fully characterized and studied for their electrical and functional properties. Experimental methods for the control of microstructure and morphology, particularly in thin films will be developed with the aid of scattering and a variety of microscopy tools including atomic force microscopy and transmission electron microscopy. Finally the newly designed materials will undergo functional testing in model configurations in transistors, light emitting diodes, photovoltaics, etc.
Major Program Achievements (over duration of support):
Since the inception of this program we have realized major advances in the development of electroactive oligomers capable of self-assembly into ordered monolayers and for which transistor function has been demonstrated. We have also developed totally novel bipolar electroactive copolymers for light emitting diodes and have demonstrated their use in highly efficient polymer-based light emitting diodes. Different copolymer architectures have been prepared and morphological studies are under way as we attempt to achieve self-ordering of the copolymers into phase separated structures in which the distance between phases is carefully tuned to achieve optimal electronic properties. We aim to develop compositions and processing protocols that afford materials capable of self-assembly into cylinders and lamellae with their axes perpendicular to the electrode surfaces. We postulate that these nanostructures will act as efficient conduits for charge transport to promote highly efficient OLED performance. We are also currently studying approaches to more sophisticated unsymmetrical or dendronized structures in which energy transfer between active moieties could be used to maximize device performance. A newly initiated program also studies the functionalization of carbon nanotubes for application in organic photovoltaic devices.
Program impact: Because novel electroactive polymers and oligomers with enhanced optimized properties hold the key to the field of plastic electronics, this program focuses on the design and synthesis of novel electroactive structures with excellent electrical properties, the control of their self-assembly into ordered structures that maximize energy efficiency; the study of factors that contribute to self-ordering and ultimate device performance, and the development of methods for optimal device construction. This program is highly interactive and multidisciplinary.
Interactions:
Internal interactions: Paul Alivisatos, Nitash Balsara, Jeff Kortright, Arun Majumdar, Howard Padmore, A. Zettl
External interactions: G. Hadziioannou (Strasbourg), V. Ganesan (UT Austin), M. Thompson (USC); M McGehee (Stanford), Intel, Nanosolar.
Recognitions, Honors and Awards: ***Segalman***: Intel Young Faculty Seed Award. ***Frechet***: 2006 Macro Group UK Medal (joint Royal Society for Chemistry and Society of Chemical Industry) for Outstanding Achievement in the field of Macromolecular Chemistry. 2005 Esselen award for Chemistry at the Service of the Public; 2005 Chemical Communications Anniversary Award; National Academy of Sciences, National Academy of Engineering, American Academy of Arts and Sciences, Fellow AAAS; American Chemical Society Award in Polymer Chemistry 2000, American Chemical Society Salute to Excellence Award 2001, American Chemical Society Cope Scholar Award 2001, American Chemical Society Award in Applied Polymer Science. *Numerous other awards and lecture series including* Baker Lecturer-Cornell, Stauffer Lecturer- Stanford, Dupont Lecturer-U Penn, Gassman Lecturer-U Minn.
Personnel Commitments for FY2005 to Nearest +/- 10%:
J. Frechet 10% (PI, program leader), R. Segalman 10% (co-PI), V. Subramanian 10% (co-PI);
L. Deng (student, 50%) B. Ma (postdoc 100%), D. Poulsen (student 50%); K. Puntambekar, (Postdoc, 100%); J. Lee, (student, 50%); B. Mattis, (student, 50%); B. Olsen (student, 50%), Y. Tao (Student, 50%), S.Y. Jang (Postdoc, 100%)
Authorized Budget (BA):
FY04 $599K FY05 $861K FY06 $861K

Laboratory Name: Lawrence Berkeley National Laboratory
B&R Code: KC020301

FWP and possible subtask under FWP: Biomolecular Materials Program
FWP Number: KC3109
Program Scope: Mimicking or application of biological materials and processes in the materials sciences. Mimicking of membranes and membrane receptors for coatings and functional interactions with living cells; of carbohydrates for controlled interface properties; of proteins for nanoscale conducting wires and self-assembling building blocks for functional assemblies; of DNA and dendrimers for 3-D patterning of inorganic nanocrystals, and as components of functional assemblies.
Major Program Achievements (over duration of support): Biosensors that turn color in the presence of agents such as influenza virus, botulinum toxin (*Bednarski/Charych*). Development of ultrasensitive SQUID based biosensors for pathogens (*Alper/Clarke*). Polymers that significantly improve the stability of proteins in unbuffered solutions and at elevated temperatures (*Bednarski*). Development of catalytic antibodies. Systems to insert non-natural amino acids into proteins (*Schultz*). The effect of specific amino acid substitutions on proteins temperature stability (*Kirsch*). Enzyme mechanisms for discrimination between optical isomers (*Koshland*). Methods for interfacing biological materials with synthetic materials. New approach for modifying carbon nanotubes with biocompatible coatings. Development of a nanoinjector for penetrating cell membranes with cargo (*Bertozzi*). Methods for isolating gold nanocrystals bearing discrete numbers of DNA oligonucleotides and the preparation of dimers and trimers of these DNA-nanocrystal assemblies and a wide variety of other spatial arrangements of nanocrystals. Discrete quantum dot Au assemblies and Au nanocrystal spectroscopic plasmon ruler (*Alivisatos*). A series of unnatural building blocks to enable automated preparation of self-assembling dendritic materials based on DNA base pairing. Preparation of dendritic "nanoreactors" that mimic the catalytic function of enzymes effecting both catalysis and transport in solution (*Fréchet*). Well defined assemblies of nanocrystals in specific arrangements (*Fréchet/Alivisatos*). Modification of natural products to allow the attachment of actin fibers to inorganic surfaces for rudimentary circuit construction. Attachment of polymers and other molecules to the viral coat protein as building blocks for complex structures. Functionalization of tobacco mosaic virus coat proteins to allow the construction of linear artificial light harvesting systems. Chemical modification of spherical viral capsids to provide versatile platforms for diagnostic imaging. Efficient chemical strategies for the modification of protein building blocks (*Francis*). A system to deliver biological molecules to prepatterned membrane structures using targeted membrane fusion. Activation of neurons from synthetic supported membranes and use of nanopatterned hybrid inorganic/organic membrane interfaces to repattern a synapse with a living Tcell (*Science* Nov. 18, 2005). Application of *in situ* photolithographic patterning technology to membrane patterning on colloidal particles (*Adv. Mats.* 2005). Use of membrane coated colloidal particles as sensitive detection assay (*Nature* 2004). Broadly scalable strategy for constructing synthetic cell membrane surfaces displaying natural cell surface proteins with genetically encoded fluorescent markers (*Groves*).
Program Impact: Biosensors for study by industry/government for military/civilian use. Expanded capability to modify enzymes for novel functions. Commercial product for stabilization of proteins at high temperatures and in unbuffered solutions. Techniques for creating hybrid devices of living cells and non-living materials, and for integrating nanoscale materials into biological systems. Over 10 papers/year in major peer reviewed journals.
Interactions: C. Larabell, UCSF; L. Landweber, Princeton; N. Seeman, NYU; M. Dustin, NYU; M. Callstrom, Ohio State; A. Tomsia, R. Ritchie, K. Healy, R. Mathies, E. Isacoff, LBL and UCB; A. Zettl (LBNL/UCB), Arto Nurmikko (Brown), Harry Atwater (CalTech), Angela Belcher (MIT), Rajesh Naik (AFRL), Johnathon Trent (NASA), Chad Paavola (NASA). Colin Nuckolls (Columbia), Angela Belcher (MIT), Rajesh Naik (AFRL), Ken Raymond (UCB), Graham Fleming (UCB), Jim O'Neil (LBNL), Chad Paavola (NASA).
Recognition, Honors and Awards (at least partly attributable to support under this FWP or subtask): *Bertozzi*-Elected National Acad. Sci., Amer. Acad. Arts & Sciences, Irving Sigal Young Invest. Award-Protein Society, ACS Award-Pure Chemistry, Merck Academic Development Award, Pres. Early Career Award-Science & Engineering, MacArthur Found. Award, Camille Dreyfus Teacher-Scholar Award, Arthur Cope Scholar Award ACS. *Alivisatos*-Nat. Acad. Sci. Amer. Acad Arts and Sci. ACS Colloid and Surf. Sci. Award. Fellow, AAAS, APS, Wilson Prize-Harvard, Coblentz Award, Sloan Found. Fellow, Pres.Young Investigator, Outstanding Young Invest.-MRS, Editor-in-Chief NanoLetters, Associate Ed. Ann Rev Phys Chem, Editorial Board: J Phys Chem, Chem Phys, J Chem Phys. *Frechet*-Nat. Acad Sci, Nat Acad Engin, Amer Acad Arts Sci, ACS Award-Polymer Chem, 2006 Macro Group UK Medal (Royal Society for Chemistry and Society of Chemical Industry) for Outstanding Achievement in Macromolecular Chemistry, 2005 Esselen Award for Chemistry in the service to the public, ACS Salute to Excellence Award, ACS Cope Scholar Award, Baker Lecturer-Cornell, Stauffer Lecturer- Stanford, Dupont Lecturer-U Penn, Gassman Lecturer-U Minn. *Groves*- Searle Scholars Award, MIT TR100 (2003), Beckman Young Investigator Award (2004), ACS Langmuir Lecture Award (2005). *Francis*-Hellman Faculty Award (2004) Dreyfus Foundation Award, NSF Career Award (2004), GlaxoSmithKlein Award (2006), Noyce Prize for Excellence in Undergraduate Teaching (2006).
Personnel Commitments for FY2006 to Nearest +/-10%: Profs. M. **Alper**, P. Alivisatos, J. Fréchet, J. Groves, M. Francis, and C. Bertozzi at 10%. 5 post-docs at 100%, 5 GSRAs at 100%.
Authorized budget (BA):

FY04 $732K	**FY05** $732K	**FY06** $732K